19th ISCB International Conference (ISCBC-2013)

RECENT ADVANCES AND CURRENT TRENDS IN CHEMICAL AND BIOLOGICAL SCIENCES

2nd -5th March, 2013

Jointly organized by

Mohanlal Sukhadia University , Udaipur,313001 ,Rajasthan, India

&

Indian Society of Chemists & Biologists, Lucknow, India

SCIENTIFIC PROGRAM

Saturday, March 2, 2013

9.30 AM -11.30 PM	**Registration**	
11.30 PM-1.00 PM	**Inaugural Session**	
	Welcome Address:	**Prof. I. V. Trivedi** ,Vice-Chancellor, Mohan Lal Sukhadia University
	Introduction to ISCB:	**Dr. P.M.S. Chauhan, Gen.Secretary, ISCB.**
	Presidential Address:	**Prof. Anamik Shah, President ISCB**
	Address by Chief Guest Address by Guests of Honour	**Prof.Jyoti Chattopadhyaya**, **Professor & Chair,** Program of Chemical Biology, Dept. of Cell & Molecular Biology, Uppsala University, **Sweden** **Prof.Victor Kartsev, Russia** **Prof Michael D. Threadgill, UK** **Prof.Cynthia J. Burrows, USA** **Prof.Athina Geronikaki , Greece**
	ISCB AWARD Lectures	**ISCB LIFE TIME ACHIEVEMENT AWARD** **ISCB AWARD FOR EXCELLENCE** **ISCB YOUNG SCIENTIST AWARD**
	Vote of Thanks:	**Prof. A. K. Goswami,** Convener & Chair
1.00-2.00PM	Lunch	

Session – I

Chairpersons: Dr.S.B.Katti and Dr.Rajesh Luthra

PL-1 2.00 PM-2.30 PM	**Jyoti Chattopadhyaya**, Professor & Chair,Program of Chemical Biology, Dept. of Cell & Molecular Biology, Uppsala University,Sweden **New Free-radical Ring closure Metathesis to give Modified DNA or RNA to Potential Therapeutics or Diagnostics**
PL-2 2.30 PM-3.00 PM	**Victor Kartsev** , *InterBioScreen, PO Box 218, Moscow, 119019 Russia* **Novel Rearrangements in Targeted Synthesis of Natural Compound Analogs**
IL-1 3.00-3.20	**Cynthia J. Burrows**, University of Utah, , USA **SINGLE-MOLECULE STUDIES OF OXIDATIVE DAMAGE IN TELOMERIC G QUADRUPLEXES**
IL-2 3.20-3.40	**Brenton DeBoef**, Department of Chemistry ,University of Rhode Island ,Kingston,USA **Synthesis of C-C and C-N bonds via oxidative C-H functionalization**
IL-3 3.40-4.00	**P.M.S.Chauhan,**Medicinal and Process Chemistry Division, Central Drug Research Institute Lucknow,
IL-4 4.00-4.20	**Rachna Sadana**, ,Assistant Professor of Biology and Biochemistry, Houston, **USA** **Screening Novel Synthetic Compounds for their Cytotoxicity and Inhibition of Tubulin Polymerization**
Tea	**4.20-4.40PM**
IL-5 4.40-5.00PM	**Fernando Albericio,** Professor ,Organic Chemistry Dept. – UB, **Spain, Therapeutic Nanoconjugates**
IL-6 5.00-5.20PM	**Krishna Nand Singh,** Professor of Organic Chemistry, Department of Chemistry **Development of Some Green Protocols for Organic Synthesis**
IL-7 5.20-5.40PM	**Pratibha Mehta Luthra**, Dr. B.R. Ambedkar Centre for Biomedical Research, University of Delhi, Delhi **Design and Development of thioxothiazoles as A2A receptor antagonists in the therapy of Parkinson's Disease**

5.40 PM – 7.30 PM **Poster Session -1(Poster Numbers 1-100)**
7.30 PM – 8.30 PM **Cultural Programme**
8.30 PM **Dinner**

SESSION – II: Chairpersons: Prof Michael D. Threadgill & Dr.P.M.S.Chauhan

PL-3, 9.00 AM-9.30 AM	**René Grée,** Directeur de Recherche CNRS,Université de Rennes 1Institut des Sciences Chimiques de Rennes, CNRS UMR 6226,Avenue du Général Leclerc,35042 RENNES Cedex**, France** **Design, Synthesis and Biological Evaluation for Analogues of Bioactive Biarylic Polyphenols**
PL-4 9.30 AM-10.00 AM	**Tushar Kanti Chakraborty**, Director, CSIR-CDRI, Lucknow , India **OSDDChem: A CSIR Initiative to Connect Chemists & Biologists**
IL-8 10.00 AM -10.20 AM	**Steven E. Rokita,** Department of Chemistry,Johns Hopkins University,3400 N. Charles St., Baltimore, MD 21218, USA. **DYNAMIC AND TARGETED ALKYLATION OF DNA**
IL -9 10.20 AM-10.40 AM	**Mahesh K. Lakshman,** Professor,Department of Chemistry,The City College and The City University of New York 160 Convent Avenue, New York, NY 10031. **N-Directed C–H Bond Activation in Purines and Purine Nucleosides**
IL -10 10.40 AM-11.00	**Arun K. Shaw**, , CSIR-Central Drug Research Institute, Lucknow **Stereoselective Synthesis of Aminocytitols by Using Carbohydrate Based Building Blocks: Formal Synthesis of (+)-Conduramine E and (-)-Conduramine E**
IL -11 11.00-11.20	**Ashok K. Prasad ,**University of Delhi, Delhi **From Glucose to Modified Nucleosides, pH Sensitive Sugar-based Polymers and Crown Ethers of Importance**

Tea: 11.20 AM-11.40 PM

Session-III
Chairpersons: Prof. A. K. Goswami and Prof. Ashok K. Prasad

IL-12 11.40 AM-12.0 PM	**Donal O'Shea,**School of Chemistry & Chemical Biology,University College Dublin,Dublin, **BF_2-Azadipyrromethene Based *in vivo* Near Infrared Fluorescence Imaging Platforms**
IL-13 **12.00PM-12.20 PM**	**Athina Geronikaki** , Department of Pharmaceutical Chemistry, Aristotle University, **Greece** **Design and synthesis of novel (4/6-substituted benzo[d] thiazol-2-yl)thiazolidinone-4-ones with antimicrobial activity**
IL-14 **12.20 PM -12.40 PM**	**Anshu Dandia** , Centre of Advanced Studies, Department of Chemistry,University of Rajasthan, Jaipur- India **Green nanotechnology: Towards Synthesis of Pharmaceutically and Biologically pertinent Moieties**
IL-15 **12.40 PM-1.00PM**	**Diwan S Rawat**, *Department of Chemistry, University of Delhi, Delhi* **Antimalarial Drug Development: From Simple in vitro Screening to Lead Identification**
IL-16 **1.00-1.20PM**	**R.I. Kureshy,***Discipline of Inorganic Materials and Catalysis, Central Salt and Marine Chemicals Research Institute (CSMCRI), Council of Scientific & Industrial Research (CSIR), G. B. Marg, Bhavnagar- 364 002,* **Chiral Catalysis an Important Tool for the Synthesis of Pharmaceutically Active Molecules**

Lunch 1.20 PM - 2.20 PM

Session-IV
Chairpersons: Prof.Steven E. Rokita and Prof. Rajesh Dhakarey

IL-17 2.20 PM-2.40 PM	**Maria Laura Bolognesi,** Department of Pharmaceutical Sciences,Via BelmeloroBologna, **Italy** **Designing multitarget drugs for neurodegenerative diseases**
IL-18 2.40 PM-3.00 PM	**Tsann-Long Su,**Research Fellow,Institute of Biomedical Sciences, Academia Sinica, Taipei ,Taiwan. **Novel antitumor indolizino[6,7-*b*]indoles with multiple modes of action: DNA cross-linking and topoisomerase I and II inhibition**
IL-19 3.00 PM-3.20 PM	**Ram Vishwakarma,** Indian Institute of Integrative Medicine, Jammu, Chemical biology of GPI molecules
IL-20 3.20 PM -3.40 PM	**Barbara Zajc**, The City College and The City University of New York **Doubly Functionalizable Reagents in Protio and Fluoro Julia-Kocienski Olefination**
IL-21 3.40 PM -4.00 PM	**S.B.Katti,**Head, Medicinal and Process Chemistry Division, Central Drug Research Institute Lucknow, India **4-Aminoquinoline derivatives as antimalarial agents**
IL-22 4.00-4.20	**Vishnu K. Tandon,**Department of Chemistry, University of Lucknow, **Regio-, chemo- and Enantioselective reactions in H_2O towards synthesis of biologically active compounds**

Tea 4.20 PM -4.40 PM

Session-V
Chairpersons: Prof. Anamik Shah and Prof Mahesh K. Lakshman

IL-23 **4.40-5.00**	**S K Puri,** Division of Parasitology, CSIR-Central Drug Research Institute, Lucknow, 226001 India, **Targeting the dormant 'Hypnozoites' for malaria elimination**
IL-24 **5.00-5.20**	**Suniti Dharwadkar,**Head, Biochemistry Department, S. B.College of Science, Aurangabad-431001, (M.S.) India **Role of Biotransformation in Pharmacological Actions of Drugs and in Drug Development: Significance of Cytochrome P-450 Enzymes.**
O-1 **5.20 PM-5.30 PM**	**Indresh Kumar**, Department of Chemistry,Birla Institute of Technology and Sciences-Pilani, Pilani **An organocatalytic direct Mannich–cyclization cascade as [3+2] annulation: Asymmetric synthesis of 2,3-substituted pyrrolidines**
O-2 **5.30 PM-5.5.40 PM**	**Sandip T. Gadge,** Department of Chemistry, Institute of Chemical Technology, Matunga, Mumbai ,India. **Oxidative aminocarbonylation of terminal alkynes for the synthesis of alk-**

	2-ynamides by using palladium-on-carbon as efficient, heterogeneous, phosphine-free, and reusable catalyst
O-3 **5.40PM-5.50 PM**	**Aniruddha B. Patiland**, **,** Department of ChemistryICT Technology, Mumbai **Selective and efficient synthesis of decahedral palladiumnanoparticles and its catalytic application for Suzuki coupling reaction**
O-4 **5.50 PM-6.00 PM**	**Umakant B. Patil,** Department of Chemistry, ICT, Matunga (E), Mumbai - 400 019, India **A novel method for the synthesis of 5-subtituted 1*H*-tetrazole from Oxime and Sodium Azide**
O-5 **6.00 P M-6.10 PM**	**A. K. Gupta** and R.S. Dubey, Department of Biochemistry, Faculty of Science, Banaras Hindu University, Varanasi, **Synthesis And Evaluation Of Antioxidant Activities Of Some New 3-Substituted-2-Oxindole Derivatives**
O-6 **6.10 PM-6.20 PM**	**Vivek K. Vyas** and Manjunath Ghate, Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India, **Pharmacophore modeling, 3D QSAR, virtual screening, docking and *in silico* pharmacokinetic and toxicities prediction studies of protein kinase B (AKT β) inhibitors**
O-7 **6.20 PM-6.30 PM**	**Hardik G. Bhatt** and Paresh K. Patel, Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India, **Discovery of hiv-i integrase inhibitors: pharmacophore mapping, database searching, molecular docking, synthesis and *in silico* pharmacokinetic & toxicities prediction.**

6.30 PM-7.00PM **Industry Academia Interaction**
7.00 PM – 8.00 PM **Poster Session -II (Poster Numbers 100-200)**
8.00 PM – 8.30 PM **Cultural Programme**
8.30 PM **Dinner**

Monday, March-04-2013

SESSION –VI

Chairpersons: Prof. Jyoti Chattopadhyaya and Prof. Athina Geronikaki

PL-5 9.00 AM – 9.30 AM	**Mukund S. Chorghade,** CSO, AGN Biofuels, 14 Carlson Circle, Natick, MA 01760 **Pre-treatment of Bagasse: A Chemists' Approach to Lignin Depolymerization**
PL-6 9.30 AM – 9.50 AM	**Prof. Anil K. Singh, Vice Chancellor**,University of Allahabad,Allahabad & Professor, Department of Chemistry, IIT Bombay **A Chemical Approach to PhotobiologyBioorganic and Excited State Studies of Retinal Related Photoreceptors**
IL-25 9.50 AM - 10.10 AM	**Laurent El Kaim,** Enseignant-Chercheur,UMR 7652,DCSO (Ecole Polytechnique) Paris ,**France** **New cyclizations of Ugi and Ugi-Smiles adducts.**
IL-26 10.10 AM – 10.30 PM	**Han-Chung Wu** Institute of Cellular and Organismic Biology, Academia Sinica, Taipei 115, Taiwan **Ligand-Mediated Drug Delivery Systems for Cancer Targeted Imaging and Therapy**
IL-27 10.30 PM – 10.50 PM	**Rajiv Sharma** (Senior Vice-President Medicinal chemistry, PLSL, Mumbai **P7170, an Orally Efficacious, Anti-cancer Clinical Candidate Targeting PI3K/mTOR & ALK-1 Kinases**

Tea : 10.50 AM - 11.10 AM

Session VII

Chairpersons: Prof. Anil K. Singh & Dr.K.C.Gupta

IL-28 11.10 PM – 11.30 PM	**Sanjay Kumar** Asst. Director Medicinal chemistry,PLSL Mumbai **Liabilities in drug discovery: Medicinal chemistry perspective**
IL-29 11.30 PM – 11.50 PM	**Dalip Kumar**, Department of Chemistry, Birla Institute of Technology and Science, Pilani- 333 031, India **Design and synthesis of novel porphyrin conjugates as photochemically triggered cytotoxic agents**
IL-30 11.50-12.10	**N. H. Khan,** Discipline of Inorganic Materials and Catalysis,Central Salt and Marine Chemicals Research Institute (CSIR-CSMCRI), Bhavnagar- 364 002, Gujarat, India. **Asymmetric Strecker Reaction Catalyzed by Chiral Catalysts**
IL-31 12.10 PM - 12.30PM	**Jitendra Kumar Saxena,** Division of Biochemistry, Central Drug Research Institute, Chattar Manzil Palace, Lucknow (U.P.) India ***Plasmodium falciparum* Transketolase and Purine Nucleoside Phosphorylase: Potential Drug Targets**
IL-32 12.30 PM – 12.50 PM	**Jawahar Lal** , CSIR-Central Drug Research Institute, Lucknow – 226001, India **Preclinical pharmacokinetics and tissue distribution study of anti-tubercular azolyl phenyl cyclopropyl methane, S010-399, in rats**
IL-33 12.50-1.10	**Anand Kumar Jain** , Dept. of Pharmacology, G R Medical College, Gwalior (M P) **Twin drugs; a drug design strategy**

Lunch 1.10 PM – 2.00 PM

Session –VIII

Chairpersons: Dr.S.K.Puri and Dr. Rajiv Sharma

IL-34 2.00 PM-2.20pm	**Mohan Prasad,Ranbaxy ,** Ranbaxy Laboratories Gurgaon **Management of Impurities- a Regulatory View**
IL-35 2.20-2.40 PM	**Jibon Kotoky**, Institute of Advanced Study in Science and Technology (IASST), Guwahati, Assam, India **Microwave Mediated Green Synthesis of Gold Nanoparticles from *Adiantum philippense* and its Cytotoxicity Study** Importance of Salts and Polymorphs during Drug Discovery and Development
IL-36 2.40 PM -3.00 PM	**K.Deo**, Wockhardt , Aurangabad, MH
IL-37 **3.00-3.20** PM	**Anamik Shah** Department of Chemistry,Saurashtra University, Rajkot- 360 005 **Synthesis and pharmacology of pyranoquinoline analogues as anti-cancer promising leads**
IL-38 **3.20PM-3.40PM**	**Anil Kumar Dwivedi,** Pharmaceutics Division, CDRI, Lucknow, India **Spermicides: Local contraceptive agents**
IL-39 **3.40-4.00PM**	**N C Desai,** Dean, Faculty of Science & Head, Department of Chemistry,Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University **Small & Hybrid heterocyclic scaffolds as smart antimicrobial agents**
IL-39A **4.00PM-4.20PM**	**A.K. Goswami,**Head, Department of Chemistry,Mohanlal Sukhadia University, Udaipur
IL-39B **4.20PM-4.40**	**B.L. Ahuja**, Head, Department of Physics, Mohanlal Sukhadia University, Udaipur
O-8 **4.40PM-4.50PM**	**Kiran Bajaj**,[a,b] S.S. Panda,[a] C. Nachef[a] and A. R. Katritzky[a,]* [a]Department of Chemistry, University of Florida, Gainesville, United States of America; [b]Department of Chemistry, Rakesh P.G. College, University of Rajasthan, Pilani, Rajasthan, India **Benzotriazole Mediated Solution Phase Syntheses of *N*-protected Peptides, Hybrid peptides and their Conjugates**
 4.50 PM-5.00PM	**TEA**
O-9 **5.00PM-5.10PM**	**Rajeev Sakhuja**,[a]Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan, India; [b]Department of Medicinal Chemistry, University of Florida, [c]Center for Drug Discovery, Northeastern University, Boston, Massachusetts, **United States**. **Novel 4-Substituted 2-Dimethylaminotetralins: Synthesis and Binding Affinity at Serotonin 5-HT$_2$-type G Protein-Coupled Receptors with *In Silico* Docking Studies**
O-10 **5.10PM-5.20PM**	**Pradeep Kumar**,Medicinal & Process Chemistry Division,**CSIR-Central Drug Research Institute,** LKO **Nanotechnology and Medical Science: Challenges Ahead**

O-11 **5.20-5.30PM**	**Braja Gopal Bag,** Department of Chemistry and Chemical Technology, Vidyasagar University, West Bengal, India **Spontaneous Self-assembly of Renewable Nano-sized Triterpenoids: Formation of Fibers, Spheres and Vesicle**
O-12 **5.30PM -5.40PM**	**Ranjan Khunt**, Saurashtra University,Rajkot- (Gujarat) India **Synthesis, antitubercular evaluation and Recursive partitioning analysis of some Imidazo[1,2-a]pyridine derivatives**
O-12A **5.40PM -5.50PM**	**Sweta Sharma**, Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi, India
O-13 **5.50PM-6.00PM**	**Jyoti Singh**, &. Makarand Waikar*,**Sci-Edge Information,**STN / SciFinder / CAS Representative,Plot #53/3, C S #110, Opposite Pariijat Building, Thorat Colony Rd, Erandwane, Pune **Patent Trends in last 5 years in the area Life Style Disease**
O-14 **6.00PM -6.10PM**	**D. N. Singh*** and N. Verma,Department of Chemistry, K. S. Saket PG College, Dr. RML Avadh University Faizabad-224001, India, **Pharmacological activity of the active constituents isolated from *some medicinal plants***
O-15 **6.10PM -6.20PM**	**O.P. Sidhu[a]**, Anil Bhatia[a], Raja Roy[b,a]CSIR-National Botanical Research Institute, Rana Pratap Marg, Lucknow-226001, India **Metabolic profiling of fruits of different chemotypes of *Withania somnifera* (L) Dunal using GC-MS and NMR spectroscopy**
O-16 **6.20PM -6.30PM**	**Rakesh Kumar[a],** Dhiraj Kumar[a] and Ashok Prasad[b,a]Department of Chemistry, Kirori Mal College, University of Delhi, India **Stereocontrolled oxidative additions upon 1,4-dihydropyridines: Synthesis of hexahydrofuro[2,3-b]pyridine derivatives**
O-17 **6.30PM -6.40PM**	**Raghuvir R. S. Pissurlenkar**, Bombay College of Pharmacy, Mumbai **Engineering Techniques for QSAR of Peptides**
O-18 **6.40PM-6.50PM**	**Kartsev V.G**., **Zubenko A.A.**[1]*InterBioScreen Ltd., 119019, PO Box 218,* **New Rearrangements of Semiaminals of Natural Origin**
O-19 **6.50PM-7.00PM**	**Ritu Kapoor**, L. D. S. Yadav*,Green Synthesis Lab, Department of Chemistry, University of Allahabad, 211002, India, Organocatalytic Asymmetric Synthesis of 1,2,4-Trisubstituted Azetidines By Reductive Cyclization of Aza-Michael Adducts of Enones

7.00 PM - 8.30 PM **Poster session-III (Poster Nos. 200 onward)**
8.30 PM **Dinner**

Tuesday 5, March, 2013

SESSION –IX

Chairpersons: Prof.Barbara Zajc and Dr.K.DEO

PL-7 9.30 AM -10.00 AM	**Michael D. Threadgill**,*Medicinal Chemistry, Department of Pharmacy & Pharmacology, University of Bath, Claverton Down, BathBA2 7AY, UK.* **Design and discovery of potent inhibitors of the tankyrases, triple-function targets in the cancer cell**
IL-40 10.00 AM -10.20 AM	**Sunil K. Sharma** ,*Department of Chemistry, University of Delhi, Delhi,India* **Bio-catalytic Synthesis of Amphiphilic Polymeric and Dendritic Architectures for Biomedical Applications**
IL-41 10.20AM -10.40 AM	**Neeraj Sinha**, Senior Principal Scientist , Division of Toxicology,Central Drug Research Institute, Lucknow **Metabonomics : A Platform for Testing Toxicity**
IL-42 **10.40 AM-11.00AM**	**Ram S. Mohan**, Department of Chemistry, Illinois Wesleyan University, Bloomington, IL 61701 USA. **Environmentally friendly organic synthesis using bismuth (III) and iron (III) compounds**
IL-43 **11.00-11.20 AM**	**M. S. Shingare,** Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431 004. (M. S.) India. **Conventional vs. Non-conventional Energy Sources for Organic Transformations in Aqueous Media**
IL-44 **11.20-11.40** AM	**G. L. Talesara,** Former Professor and Head,Department of Chemistry,Mohanlal Sukhadia University, Udaipur **Target to develop chemotherapeutically potential heterocyclic class of privileged scaffolds and their combinations, prediction of their bioactivity, biological evaluation and their structure activity relationships**
IL-44A **11.40 AM-12.00 PM**	**P.P. Yadav,** MPC Division, CSIR-CDRI,Lucknow **Spiroannelated 1,2,4-trioxanes as antimalarials**
IL-44B **12.00 PM-12.20**	**Vineet Kumar,**Chemistry Division,,Forest Research institute,Dehradun, **Polysaccharides based therapeutics: Structure and Derivatization**
IL-44C 12.20 PM-12.40	**Mahip Bhatnager,** Dean University college of Science ,Mohanlal Sukhadia University, Udaipur, **Mobile phone radiations (900MHz radiofrequency): Effects on structure and physiology of brain**
O-20 **12.40AM-12.50**	**Trapti Aggarwal**, Department of Chemistry, University of Delhi, Delhi **Regioselective Synthesis of Pyrrolo[1,2-*a*]quinolines via Electrophilic Cyclization/[3 + 2] Annulation with Concomitant Ring Opening of Iodo-Pyranoquinolines**
O-21 **12.50-1.00**	**Bhawani Singh** , Department of Chemistry, Banasthali Vidyapith, Banasthali (Rajasthan)-304022 Synthesis of hetero ring condensed some Carbazoles & Azacarbazoles

1.00 PM - 1.30 PM	**Valedictory Session**
1.30 PM - 2.00 PM	**Lunch**
2.00 PM	**Sightseeing**
2.20 PM - 3.30 PM	**ISCB GENERAL BODY MEETING**

ISCBC-2013

A Book of Abstracts of 19th ISCB International Conference
Recent Advances and Current Trends in Chemical and Biological Sciences

2nd - 5th March, 2013
Udaipur, INDIA

19th ISCB International Conference (ISCBC-2013)

RECENT ADVANCES AND CURRENT TRENDS IN CHEMICAL AND BIOLOGICAL SCIENCES

2nd - 5th March, 2013

Book of Abstracts

Editors

Prof. A.K. Goswami
Prof. R.S. Chauhan

Asstt. Editor

Dr. Manoj Chhangani

Jointly Organized by
Indian Society of Chemists and Biologists (ISCB) and
Department of Chemistry, Mohanlal Sukhadia University, Udaipur
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The authors of the papers/abstracts are alone responsible for technical contents of the papers/abstracts and references therein.

Mohan Lal Sukhadia University, Udaipur

Indra Vardhan Trivedi
Vice-Chancellor

Message

It is a matter of immense pleasure to know that Department of Chemistry, Mohanlal Sukhadia University, Udaipur is organizing 19th ISCB International Conference (ISCBC-2013) on "Recent Advances and Current Trends in Chemical and Biological Sciences during 2-5 March, 2013 and also publishing a Souvenir on this occasion.

I am sure that four day conference shall provide a common platform for a large number of participants to exchange their views, identify priority areas of future research, add something to the knowledge of all participants and stir the young minds to come up with some creative and novel ideas of research in this field.

I convey my heartfelt best wishes to the organizers for the Conference and publication of the Souvenir.

I wish the conference a great success.

(I.V. Trivedi)

From the desk of

ISCB President and General Secretary

Prof. Anamik Shah **Dr. P.M.S. Chauhan**

We are extremely happy that **Indian Society of Chemists and Biologists** is organizing its 19th International Conference (ISCBC-2013), 2nd -5th March, 2013 on **"Recent Advances and Current trends in Chemical and Biological sciences"** at Mohanlal Sukhadia University, Udaipur.

19th International conference (ISCBC-2013) at Udaipur has prime objective to provide an opportunity for a close interaction of scientists with varied interests in diverse fields of the research. This conference will also provide common platform and more opportunities to the researchers in the areas of chemical sciences and biological sciences and other related areas to interact with each other. This will also provide a forum for in-depth assessment of the challenges involved in the dynamic and fast moving field of Drug research. It will bring together leading Chemists, medicinal chemists, pharmacologists, biotechnologists, and other allied professionals to discuss and present the latest important developments in Chemical and Biological sciences .

We are glad that the scientific committee is bringing out CD and a book of abstracts covering the presentation to be made during ISCBC-2013**.** Our sincere thanks are due to the members organizing committee. During this conference a number of eminent scientists and technologists of the country and overseas will be discussing the trends, prospects and future directions of research. We look forward to fruitful deliberations in extremely interesting areas of scientific research. We are happy that an extensive and comprehensive scientific program is arranged. The scientific program beside inaugural function includes plenary lectures, invited lectures by the eminent scientists from India and abroad. Oral presentations by the young researchers are scheduled. The most heartening feature of the conference is that it is being participated with a number of young scientists and Ph. D. students and presentations are schedules in poster sessions. We are looking to the galaxy of speakers and young participants who made this conference a memorable event. We extend our warm welcome to all national and International delegates from pharmaceutical companies, research organization, universities and academic institutes wish them very happy stay at Udaipur. Now Finally I take this opportunity to express my sincere thanks and gratitude to members and office bearers of organizing committee of 19th International Conference (ISCBC-2013).

(Prof. Anamik Shah)
President, ISCB

(Dr. P.M.S. Chauhan)
General Secretary ISCB

Department of Chemistry
Mohan Lal Sukhadia University, Udaipur

Dr. A.K. Goswami
Prof. and Head

Message

It is matter of great delight that 19th ISCB International Conference is being organized by Department of Chemistry, Mohanlal Sukhadia University, Udaipur. We are privileged to have this great opportunity to exchange views with renowned scientists in the field of chemistry and biology. It is indeed a platform where well known research leaders of the world would deliberate and project their findings which would definitely immensely benefit research workers of our country.

I am happy that our researchers would interact with the global research leaders and thus would be benefited from the conference. There is no doubt the co-ordination team of our department and faculty has put lot of their effort to make this event a great success.

I wish conference a great success and congratulate the organizers and society.

(Prof. A. K. Goswami)
Convener & Chair
ISCBC-2013

From the desk of editor

I am happy to announce the publication of book of abstract for 19th ISCB International Conference (ISCBC-2013), which is held from 2-5 March, 2013.

The enthusiastic response in the form of more than 500 presentations and 54 knowledgeable lectures reflects very high scientific as well as academic level of the conference.

It had been difficult to format this huge number of abstracts but undaunted support by our team of dedicated research scholars and students has made it possible to release this compilation well in time. Still we may have committed some errors for which no one other than us are responsible. However, we have tried our every best to make this book of abstract as flawless as possible.

I wish the participants and delegate a very comfortable stay and memorable time in the 'City of Lakes'.

(Prof. R.S.Chauhan)
Organizing Secretary
ISCBC-2013

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Keynote

Dr. Marinda Li Wu

President of the American Chemical Society,USA

Dr. Marinda Li Wu received a B.S. *cum laude with Distinction in Chemistry* from the Ohio State University in 1971 and a Ph.D. in Inorganic Chemistry from the University of Illinois in 1976. With over thirty years of experience working in the chemical industry, she enjoyed many years working for Dow Chemical R&D as well as Dow Plastics Marketing forging partnerships between industry, education, government and communities. Dr. Wu also has entrepreneurial experience with various small chemical companies and startups including *"Science is Fun!"* which she founded to engage young students in the excitement of science and enhance public awareness of the importance of supporting and improving science education.

As an ACS member for over forty years, Dr. Wu has served in many leadership roles at boththe local and national levels for the American Chemical Society. Dr. Wu was elected to the ACS Board of Directors and served as Director-at-Large since 2006.In 2011, she was elected to the Presidential succession of the American Chemical Society. As ACS President-Elect for 2012, she gave lectures worldwide and was awarded various medals and made an honorary member of the Romanian Chemical Society and Polish Chemical Society. She serves as ACS President in 2013 and Immediate Past President in 2014.

Partners for Progress and Prosperity

Marinda Li Wu

2013 President of the American Chemical Society,USA
Email: marindawu@gmail.com

The global chemistry enterprise faces numerous challenges today -- the public's persistent negative perception of the chemical industry, widespread science illiteracy, increasing competition for funding and good jobs, plus the need for efficient alternative energy, clean water and air, and accessible medicines. In view of these factors, it makes sense to work together for mutual benefit as part of the international scientific community, addressing these global challenges and seeking opportunities for advancement.

We may have different languages and cultural backgrounds, different governmental and industrial organizations, and perhaps different educational systems, but we all bring unique strengths and valuable perspectives to the enterprise. We should communicate and explore initiatives to better position the global chemistry enterprise for the future. Examples of collaborative projects include better publicity for chemistry, joint educational or research programs, as well as promising technologies and business opportunities to address pressing scientific and technological issues. Through partnerships and collaborations, we can all contribute, make progress, and prosper together in the global chemistry enterprise of the future.

PL-1

Professor Jyoti Chattopadhyaya,

Uppsala University, Sweden

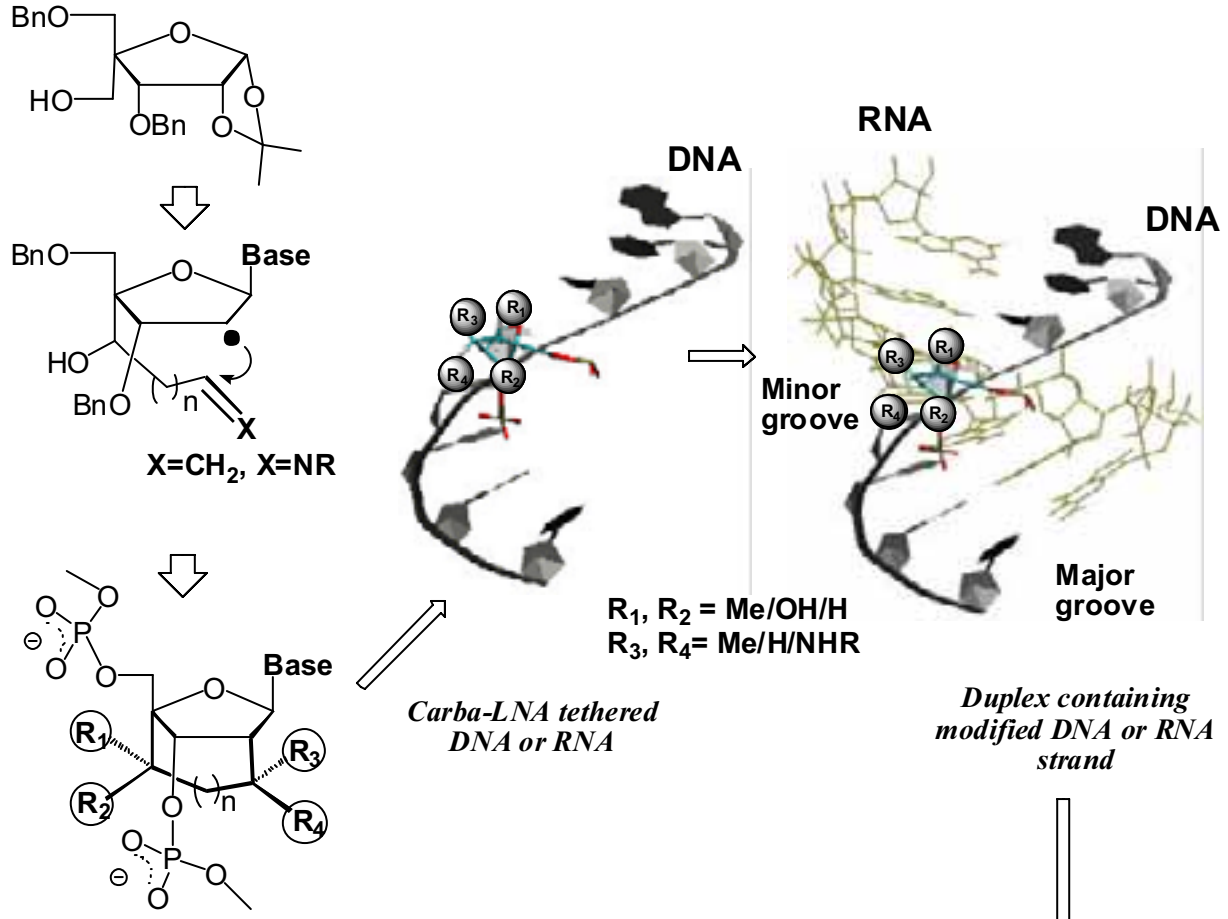
Professor Jyoti Chattopadhyaya is a Chair of Bioorganic Chemistry and is also Program Director of the Chemical Biology at the Department of Cell & Molecular Biology at the University of Uppsala, Sweden. The first program of Bioorganic Chemistry has been established by him in Sweden back in 1980, and since than he has supervised research of 30 Ph.Ds, promoted 3 Docents, and has reported high level Bioorganic chemistry research, resulting in over 410 publications in various peer-reviewed Journals **(for details of his publications, see http://www.boc.uu.se)**.

Prof. Chattopadhyaya is leading multidisciplinary research at the interface of the frontiers of synthetic and physical chemistry/Structure/Enzymology. His research focuses on (a) design of *gene (RNA)-directed therapeutics* based on Antisense oligonucleotides, Small interfering RNA (siRNA) and micro-RNA, in which the translation of the RNA specific to a gene is selectively inhibited, thereby arresting the expression of undesireable protein. (b) Physical and structural chemistry of DNA and RNA foldings by high-field multinuclear NMR spectroscopy. (c) design and synthesis of drug against *resistant bacteria* including hospital infections – MDR and XDR *Tuberculosis*, *Staphylococcus aureus* (both methicillin and penicillin resistant), vancomycin resistant *Enterococcus* and pseudomonas. In these research he employs synthetic organic chemistry of heterocycles carbohydrates and phosphorus to design mimics to model biological functions and the transition state biological intermediates. His major achievements include (a) successful design of new conformationally-locked chemically modified nucleo(s)tides to self-organize oligo-DNA and –RNA molecules to minimize the contribution of entropic energy penalty to the free-energy, (b) to improve the stability and cellular *delivery* of siRNAs and antisense oligonucleotides; (c) development of new synthetic methodologies for RNA, DNA, and carbohydrates and their modified analogs as potential DNA/RNA-directed therapeutics (siRNAs, antisense, triplexing agent, aptamers, etc), including synthetic and physico-chemical aspects of monosaccharide, heterocyclic, and phospholipid, phosphorylating and protecting group chemistry. (d) development of novel active antibiotic lead compounds against multiple drug resistant and extensive drug resistant strains of tuberculosis and hospital pathogens; (e) determination of NMR solution structures of RNA to understand RNA folding-dependent function of non-coding RNAs with emphasis on the role of microRNA, siRNAs and RNA catalyst; (f) elucidation of bioorganic chemical mechanisms using synthetic physical and structural (NMR) chemistry to model transition state or the intermediate of biochemical reactions, such as splicing, RNA catalysis, and RNA-RNA-ligand or RNA-DNA-ligand interactions; (f) development of new chemical tools for RNA, carbohydrate and peptide synthesis to understand molecular details of how structure of molecules dictate function.

New Free-radical Ring closure Metathesis to give Modified DNA or RNA to Potential Therapeutics or Diagnostics

Jyoti Chattopadhyaya

Chemical Biology Program, Department of Cell and Molecular Biology,Biomedical Center, Uppsala University, SE-751 23 Uppsala, Sweden; email:jyoti@boc.uu.se



Application:
1) New Potential Therapeutic
2) New Diagnostic
3) Bypass Multiple Resistance Problems generally encountered in protein targeting antibiotics

Examine:
1) Stop RNA translation to Protein
2) Specific Gene knock-down
3) Synthetic Biology, in general

See "Intramolecular Free-Radical Cyclization Reactions on Pentose-Sugars for the Synthesis of carba-LNA and carba-ENA and the Application of Their Modified Oligonucleotides as Potential RNA Targeted Therapeutics." C. Zhou and J. Chattopadhyaya. *Chemical Reviews,* 112 (7), 3808−3832 (2012). For full list of publications see http://www.boc.uu.se.

JC thanks all of his present and past co-workers whose names appear in the publication list.

PL-2

Professor Victor Kartsev

(Professor Dr., academician of RANS)
(e-mail: vkartsev@ibscreen.chg.ru , www.ibscreen.com, www.cbcconf.com)

Chairman of the Board of Directors of InterBioScreen Ltd. Chairman of the Board of the International Scientific Partnership Foundation and Cultural Heritage Foundation. An internationally recognized Russian scientist, author of more than 400 research publications and inventions, co-author and editor of 30 scientific monographs.

Scientific interests are in the area of chemistry of biologically active heterocyclic compounds and pharmaceuticals, chemistry of natural products. As a Head of Interbioscreen Ltd., over 18 years has been in charge of research programs and contract research projects pursued by >3000 CIS scientists in cooperation with over 700 leading pharmaceutical and biotechnology companies in Europe, US, Canada, Japan, South Korea in their quest for new highly effective pharmaceuticals and agrochemicals. Leader of several International Projects undertaken jointly with pharmaceutical and agrochemical companies, universities and research centers.

Date of birth: 01.10.1950 Place of birth: Pavlograd, Ukraine

Education:

1967-1972 – Lomonosov Moscow State University and Moscow Universirty post-graduate course
1972 – defended PhD. thesis
1987 – defended Doctor of Sciences thesis

Professional experinece:

1991 – President of SYNTEST Ltd. and SYNTEST-Princeton Ltd.
1995 – until present – Chairman of the Board of Directors (CEO) of "Interbioscreen Ltd.",
2001 – until present – Chairman of the Board of "Scientific Partnership Foundation"
2007 – until present – Chairman of the Board of "Cultural Heritage Foundation"

Awards:

2012 – Gold Medal of Peter I «For merits in the revival of science and economy of Russia"
2011 – Honorary full member (Academician) of the Russian Academy of Arts
2011 – Medal «For contribution to the culture of Ukraine» (Foundation of Culture of Ukraine, Kiev)
2010 – Academician N.M.Emanuel Medal for scientific achievements (Russian Academy of Sciences & Lomonosov Moscow State University)
2010 – Prof.A.N.Kost Medal for achievements in Chemistry of Heterocycles (Moscow University, Mendeleev Chemical Society, ISPF)
2010 – Full member (Academician) of Peter-the-Great Academy of Sciences and Arts
2009 – P.Tret'yakov Medal "For support of traditions in art", IASS, RANS
2008 – Award " The Knight of science and arts ", Russian Academy of Natural Sciences
2008 – Vernadski Medal for the scientific Achievements (RANS)
2008 – Member of the Presidium of Russian Academy of Natural Sciences
2007 – Full member (academician) of Russian Academy of Natural Sciences

2006 – **"European Falcon Award" and Diploma of the Honorary Membership of the International Association for European Cooperation and Integration**

2005 – **Grand Prix Europeen de la Qualite, Medal and Diploma, Geneva, Switzerland**

2004 – **Diplomas in two nominations: "The best manager" and "The best company", 5th Russian Venture Fair, S.-Petersburg, Russia**

2004 – **Diploma "Honorary Lifetime Membership", Indian Society of Chemists and Biologists**

2004 – **Diploma "A Lifetime Membership", Egyptian Heterocyclic Chemical Society**

2002 – **Award of EuroUnion "Viennese cup" in two nominations : "Organization of XXI century" for Scientific Partnership Foundation and personal award "Manager of XXI century"**

2001 – **Gold Medal awarded by Societe d'Encouragement pour l'Industrie National, France**

1985 – **Gold Medal at the Exhibition of Achievements of a National Economy**

1984 – **Gold Medal awarded by VDNKH**

1983 – **Laureate of the USSR State Komsomol Prize in the area of organic chemistry and biochemistry**

1972 – **Nominal Medal awarded by the Academy of Sciences of the USSR**

1970 – **Silver medal awarded by Ministry of Higher Education of the USSR**

1967 – **Honor Gold Medal for Academic Excellence (High School)**

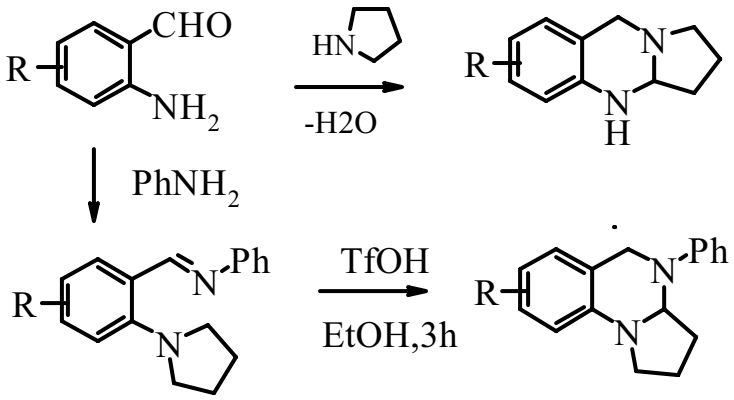
PL-2

Novel Rearrangements in Targeted: Synthesis of Natural Compound Analogs

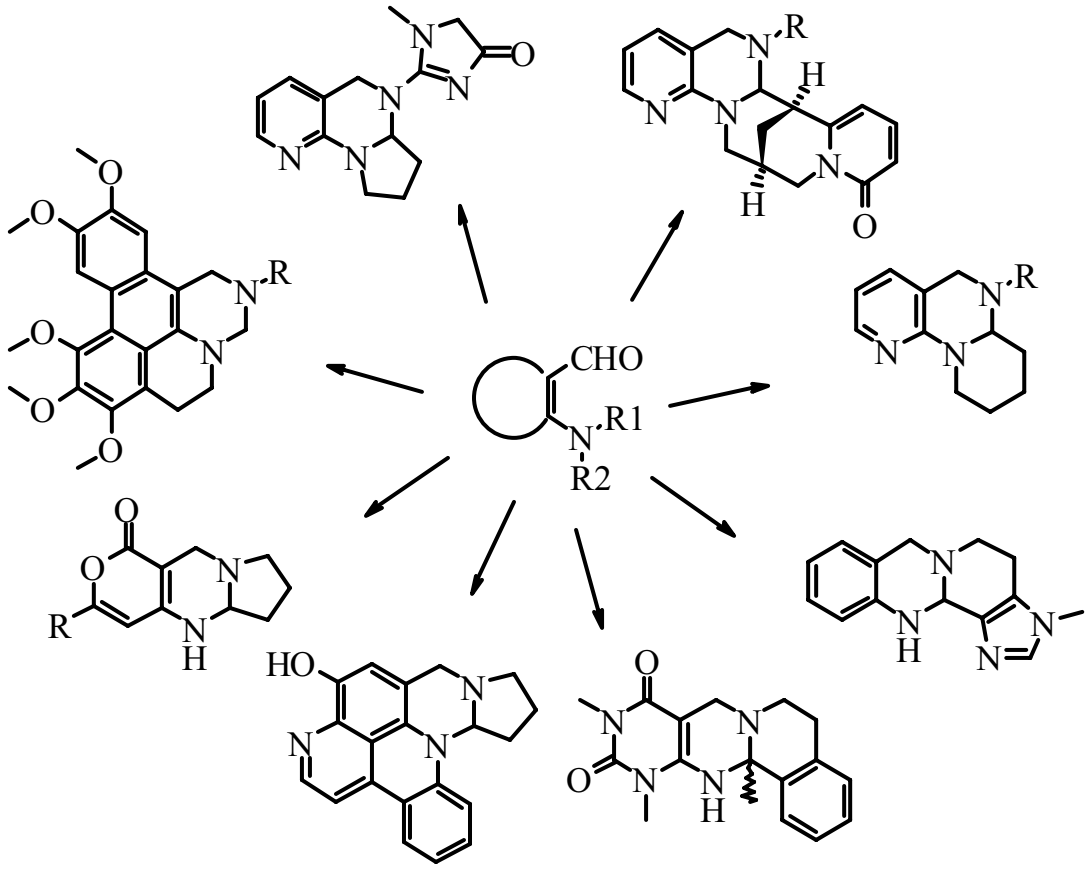
Victor Kartsev

InterBioScreen, PO Box 218, Moscow, 119019 Russia, screen@ibscreen.chg.ru

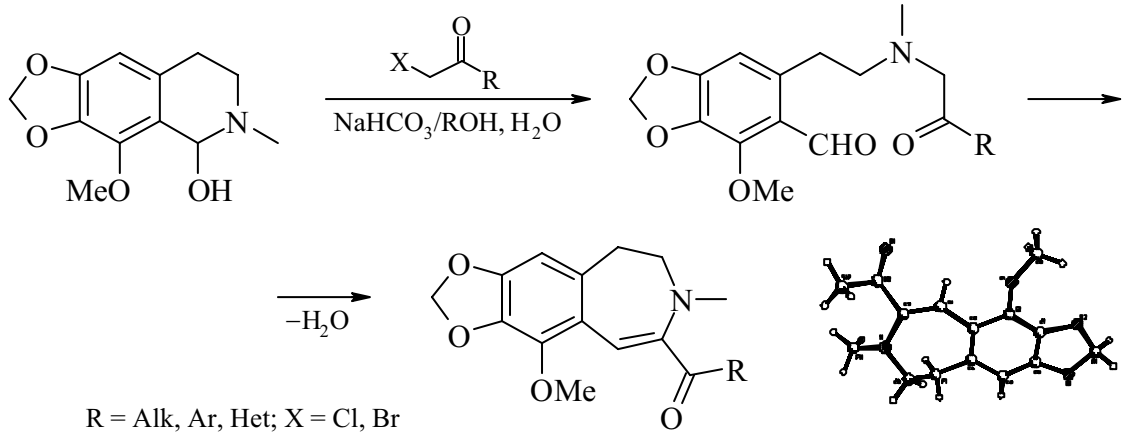
In their 2008 paper, Daniel Seidel *et al*.[1] described the reaction of ?-aminobenzaldehyde derivatives with secondary and primary amines which leads to the formation of cyclic aminals. The reaction has been a versatile tool for the synthesis of condensed heterocyclic systems:



We have extended such reactions to the synthesis of new complex heterocyclic systems on the basis of synthetic and natural ?-aminobenzaldehydes [2]:

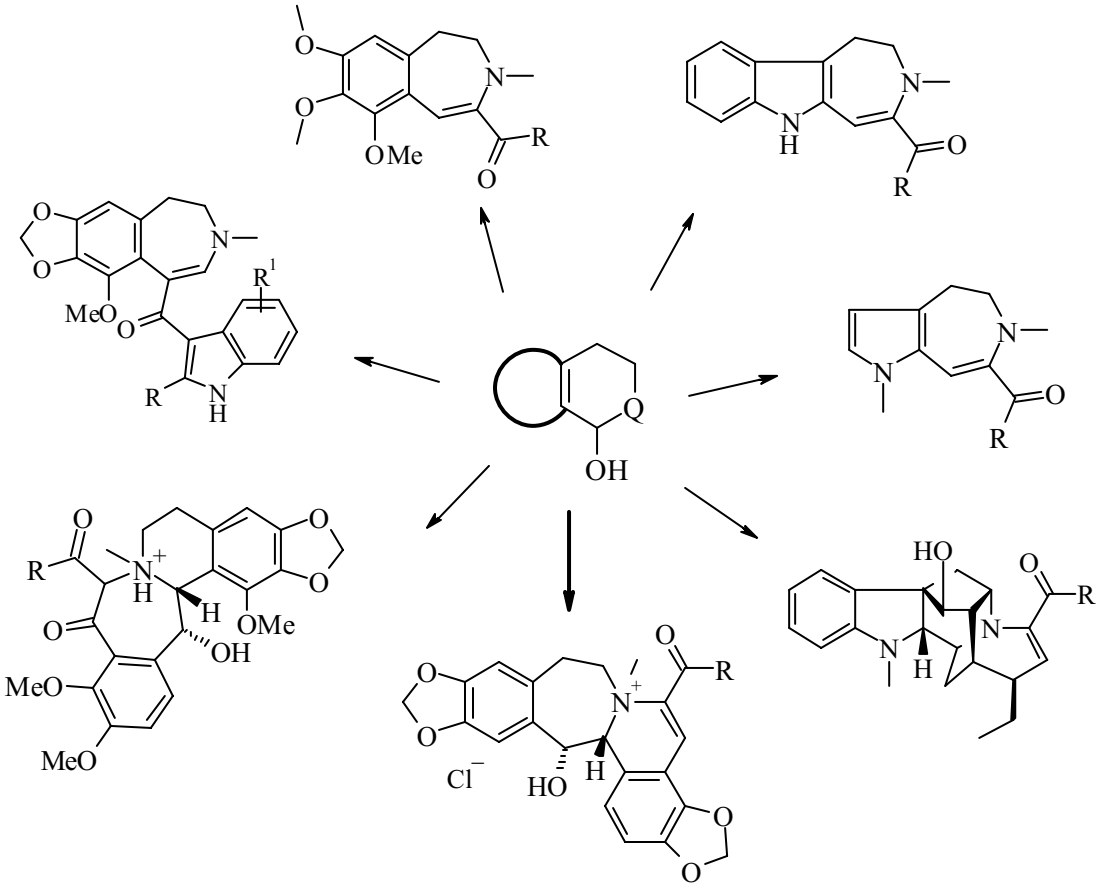


In the course of the study of alkaloid Cotarnine transformations [3] we have found that in the interaction of the Cotarnine base and its natural analogs there take place rearrangements with the formation of benzazepine systems [4]:



R = Alk, Ar, Het; X = Cl, Br

Taking various hemiaminals as an example it has been shown that the rearrangement proceeds by the general pattern which makes it possible to carry out directional synthesis of the most diverse heterocycles representing mimetics and analogs of rare alkaloids with a high bioactivity:



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2. Kartsev V.G. *et al*., in *New Aspects of Heterocyclic Chemistry, Ed. Kartsev V.G*., ? os?ow: ICSPF Press, **2010**, 273; 279.
3. Krasnov K.A, Kartsev V.G., Khrustalev V.N., *Heterocycles* **2007,** *Vol.71, ? 1,* 13.
4. Kartsev V.G. *et al*., in *New Aspects of Heterocyclic Chemistry, Ed. Kartsev V.G*., ? os?ow: ICSPF Press, **2010**, 84.

PL-3

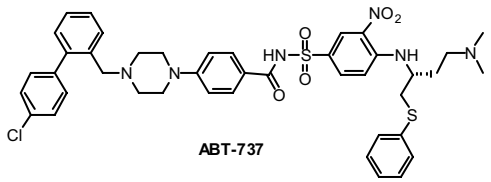
Name	Dr. GREE René
Birthdate	March 5, 1948 (Rennes, France)
Professional Address	Laboratoire Sciences Chimiques de Rennes (SCR) CNRS UMR 6226 Université de Rennes 1 Avenue du Général Leclerc, 35042 RENNES-Cedex, FRANCE Tél: (33) (0)2 23 23 57 15 Fax : (33) (0)2 23 23 69 78 E-mail: rene.gree@univ-rennes1.fr
Qualifications	Ph.d. Thesis, University of Rennes (advisor: Prof. R. Carrié, 1975) post-doctoral, Ohio State University Columbus(advisor: Prof. L.A. Paquette, 1977)
Present Position:	Directeur de Recherches Classe Exceptionnelle CNRS (equivalent to full Professor) Codirector of the Indo-French "*Joint Laboratory for Sustainable Chemistry at Interfaces*" (LIA CNRS-UR1/IICT-CSIR India)
Awards and Honours	Organic Chemistry Division Award of the French Chemical Society (1985) Elected Maître de Conférences (Part time Lecturer), Ecole Polytechnique,Paris (1990-2002)
Present Research Interests	Organometallic chemistry and catalysis directed towards organic synthesis Fluorine Chemistry Medicinal chemistry (cancer, diabetes, CNS) Chemistry in, and with, Ionic liquids
Scientific results	225 publications in international scientific journals Supervision of 50 phD thesis and 20 postdocs Over 220 invited seminars and lectures, in France and many foreign countries including over 40 plenary lectures in international congress
Scientific Commitees	French representative for the COST D2 Action (selective synthesis) at the European Community, Brussels (1972-77) Elected member of the CNRS committee for Organic Chemistry (1992-95) *President* of the CNRS committee for Organic Chemistry (1995-2000)
Editorial Boards	6 international journals
Consultantship	5 industrial laboratories (chemistry and pharmacy)

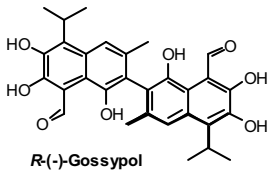
Design, Synthesis and Biological Evaluation for Analogues of Bioactive Biarylic Polyphenols

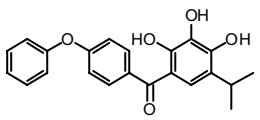
R. Grée

Université de Rennes1, Institut des Sciences Chimiques de Rennes,
CNRS UMR 6226, Avenue du Général Leclerc, 35042 Rennes-Cedex, France and
"Joint Laboratory for Sustainable Chemistry at Interfaces"
(LIA CNRS-UR1/IICT-CSIR India
Email: rene.gree@univ-rennes1.fr

Apoptosis is one of the major cell death pathways involved in maintaining cell homeostasis and so, escape from apoptosis contributes to carcinogenesis. The antiapoptotic Bcl-2 proteins are frequently overexpressed in cancer cells, including solid tumors. Current data indicate that they contribute to the aberrant survival and/or maintenance of cancer cells by counteracting death signals triggered by oncogenic lesions and/or therapy. Thus, antiapoptotic Bcl-2 proteins inhibitory strategies are of therapeutic interest. For instance, ABT-737 is a representative example of a small molecule inhibitor, which induces apoptosis in some cancer cells as a single agent or enhances the proapoptotic activity of other drugs, both *in vitro* and *in vivo*. The polyphenol core is widely recognized as an attractive structure-target towards new anticancer agents. For instance, Gossypol showed very good activities towards Bcl-2, Bcl-xL and Mcl-1. Various molecules based on the Gossypol structure were designed, for example the benzophenone derivative **1** and several analogues.







Selected inhibitors of Bcl-2 proteins

As part of our ongoing programme on the development of anticancer molecules based on reinduction of apoptosis in cancer cells, we designed and prepared new polyphenol-derived molecules which have been submitted to a biological screening. Results of these studies will be presented during the conference.

PL-4

Tushar Kanti Chakraborty

FNA, FASc, FNASc, JC Bose Fellow, CSIR-Central Drug Research Institute, Lucknow, India
Email: chakraborty@cdri.res.in
Website: http://www.cdriindia.org

Graduated in 1979 from IIT Kanpur, obtained his Ph.D. in chemistry from the same institute in 1984 and subsequently held postdoctoral position at University of Pennsylvania, Philadelphia prior to joining IICT Hyderabad in 1987. Since December 2008, he is in CSIR-Central Drug Research Institute, Lucknow. His research interests lie in the areas of organic synthesis, peptides and peptidomimetics, designing new amide-linked molecules based on sugar amino acids and related compounds and studying their three-dimensional structures and properties.

He is elected Fellows of the Indian National Science Academy, Indian Academy of Sciences, and the National Academy of Sciences, India, and has been awarded Shanti Swarup Bhatnagar prize, NASI-Reliance Industries Platinum Jubilee Award, JC Bose Fellowship, Pt. Jawaharlal Nehru National Award in Science by Madhya Pradesh Council of Science & Technology, Andhra Pradesh Scientist Award, etc.

OSDDChem: A CSIR Initiative to Connect Chemists & Biologists

Tushar Kanti Chakraborty

CSIR-Central Drug Research Institute, Lucknow, India

Synthesis of structurally complex and biologically active natural products remains as fascinating and challenging as ever. India's R&D strengths in the last few decades have been in the fields of organic synthesis, purification, extraction and structure elucidation of small molecules. This has powered India to be a world leader in the production of generics and a provider of affordable drugs the world over. Our success in organic synthesis has also given us the confidence to venture into the emerging areas of creating new molecular entities. We are well endowed today to create in the laboratory diverse arrays of new molecules with tailor-made structures and properties. The challenges are to find ways to quickly assemble complex three dimensional drug-like structures that can be easily scaled up for drug developmental purposes.

Many natural products as well as synthetic designer molecules are being made in large number of laboratories in the country which can have potential therapeutic applications. The lecture will discuss the ways that India can make progress from being one of the largest producers of generics to its coming of age initiating new drug development programs, especially for diseases prevalent in the country. OSDDChem, a CSIR initiative under the OSDD umbrella envisions achieving this objective by bringing together the synthetic chemists and the very able biologists present in the academic and research institutes in the country in a common platform to work toward a common goal.

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PL-5

Pre-treatment of Bagasse: A Chemists' Approach to Lignin Depolymerization

Mukund S. Chorghade

CSO, AGN Biofuels, 14 Carlson Circle, Natick, MA 01760

AgroGreen Biofuels (AGN) has developed innovative, cost-effective, proprietary technology solutions for pre-treatment of biomass with synthetic catalysts for effective depolymerization of lignin. AGN has synthesized, efficient, sterically protected and electronically activated organic biomimetic catalysts that depolymerize lignin, at ambient temperatures and pressures, to a mixture of phenolics, hemicellulose and cellulose in excellent yield.

Salient features of our technology include:

- Structural scaffolds incorporate the aza macrocycle into the primary structure.
- Depolymerization of lignin is complete in primarily aqueous systems; limited amounts of organic solvents are used. The co-oxidants that are used are effective in neutral to mildly alkaline conditions, and the pH is maintained at this level throughout.
- Reduction/elimination of enzyme in saccharification through in-situ enzyme productionwith recombinant microbes further reduces the overall production cost
- Use of plant waste that is geographically abundant and available locally to minimize transportation costs

In addition we have optimized product yields by

- Improving enzyme efficiency across different environments (pH and temperature)
- Genetically modified efficient microbes to gain higher yield in the fermentation process
- Adopted Sustainable and Eco-Friendly Alternatives
- Used a wide variety of plant waste as a feedstock

PL-6

A Chemical Approach to Photobiology
Bioorganic and Excited State Studies of Retinal Related Photoreceptors

Anil K. Singh

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai; University of Allahabad, Allahabad
e-Mail: <Retinal@chem.iitb.ac.in,<vc_au@allduniv.ac.in>

Photobiology is a multidisciplinary area that deals with the study of the effects of light on living organisms and ecosystems. Topics like photosynthesis, vision, photoperiodism, photomorphogenesis, bio- and chemiluminescence, photomedicine, environmental photobiology, ultraviolet radiation effects, phototechnology, etc. are commonly studied in photobiology. As new biology seeks to understand all of the processes of life at the molecular level, researchers have tried to use the concepts and tools of photobiology to develop molecular level understanding of many light-induced biological processes that occur in the Nature. Such knowledge in turn has influenced many areas of science and technology dealing with sensory biology, electronics and communication, human health, agriculture, global climate and environmental changes, energy, and many other areas of human concern. Several types of sensory (*e.g.* vision) and energy transductions (*e.g.* ion-transport) in living systems are mediated by protein-based photoreceptors containing retinal as the chromophore. Rhodopsins (*e.g.* visual pigment rhodopsin and halobacterial pigment bacteriorhodopsin) are the prime examples of such photoreceptors. Bioorganic and excited state studies of rhodopsins and their models have helped to unravel the molecular details of the structure and mechanism of functions of these photoreceptors. In particular, such studies have been very useful in understanding the chemical nature of the primary events that occur in the photoreceptor soon after absorption of light, and the interactions that occur between the chromophore and the surrounding protein residues. These studies have also paved way for design of analog systems, with altered electro-optical properties, and new strategies to design photoswitches for various biological, chemical, electronic and medical applications.

PL-7

Prof. Michael D. Threadgill

Head of Medicinal Chemistry
Department of Pharmacy & Pharmacology, University of Bath, Membership of professional societies

Fellow of the Royal Society of Chemistry (FRSC, CChem) since April 1994; International Society for Heterocyclic Chemistry; Association for Radiation Research; Society for Medicines Research; British Association for Cancer Research.

Supervision and support for postgraduate research students

29 Students supervised to completion and award of PhD; 1 student supervised to completion and award of MPhil.

University Ombudsman for Postgraduate Research Students for the University of Bath (since 2003).

Publications

130 Full papers in peer-reviewed scientific journals; 9 reviews in peer-reviewed scientific journals; 2 patents.

Current research interests and group

Medicinal chemistry applied to problems in cancer and other diseases. Design, synthesis and evaluation of inhibitors of enzymes: sirtuins, poly(ADP-ribose)polymerases (PARPs), tankyrases, dihydrofolate reductase of *M. tuberculosis*. Polymeric prodrug systems for selective delivery to prostate tumours.

Inhibition of tankyrases: One postdoctoral researcher and two PhD students (funded by AICR and University of Bath)

Inhibition of DHFR of M. tuberculosis: One PhD student (funded by Saudi Government)

Polymeric prodrugs: One PhD student (funded by Prostate Cancer Charity).

Design and discovery of potent inhibitors of the tankyrases, triple-function targets in the cancer cell

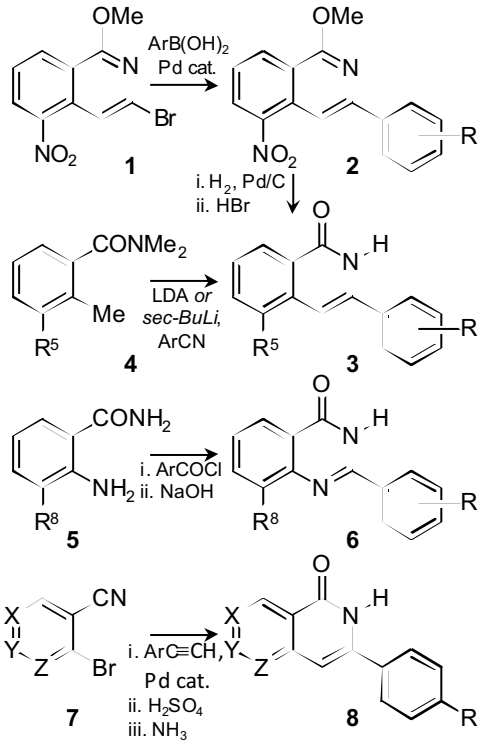
Michael D. Threadgill,* Amit Nathubhai, Helen A. Paine, Katerina Kumpan, Pauline J. Wood, Matthew D. Lloyd and Andrew S. Thompson

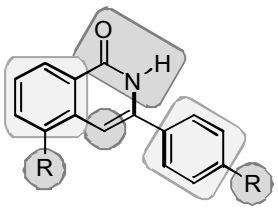
Medicinal Chemistry, Department of Pharmacy & Pharmacology, University of Bath, Claverton Down, BathBA2 7AY, UK.

m.d.threadgill@bath.ac.uk

Tankyrases-1 and -2 are members of the poly(ADP- ribose) polymerase (PARP) enzyme superfamily. They regulate target proteins through transfer of multiple ADP-ribose units from substrate NAD^+, building a short polyanionic polymer [1,2]. Unlike PARPs-1 and -2, which are implicated in DNA repair, tankyrases-1 and -2 have unique cellular roles, including the regulation of elongation of telomeres [3], the activity of NuMA in mitosis [3] and the *Wnt* signalling pathway [4]. All three of these are attractive in developing new anti-cancer drugs.

Using the published crystal structures of tankyrases-1 and -2 and building on our library of inhibitors of PARPs-1 and -2,[5] we designed several series of 3-arylisoquinolin-1-ones, 2-arylquinazolin-1-ones, arylnaphthyridinones and arylpyridopyrimidinones. The key step in synthesis of the 5-amino-3-arylisoquinolin-4-ones **3** ($R^5 = NH_2$) was Suzuki coupling of bromo isoquinoline **1** with arylboronic acids, whereas the 5-methyl-, 5-methoxy- and 5-fluoro- 3-arylisoquinolin-1-ones **3** (R^5 = Me, MeO, F) were approached by reaction of the carbanion derived from 3-substituted 2,N,N-trimethylbenzamides with the appropriate benzonitrile. Most of the quinazolin-4-ones **6** were obtained by acylation of anthranilamides **5** and cyclisation under basic conditions. The naphthyridinones **8** (X or Y or Z = N) were formed by Sonogashira reaction of the corresponding bromopyridinenitrile **7**, acid-catalysed 6-*endo*-dig cyclisation and treatment with ammonia under pressure.





Pharmacophore for inhibition of tankyrases

Compounds were evaluated for inhibition of auto-poly(ADP-ribosyl)ation of tankyrase-2, using an assay developed in-house. With some examples showing apparent IC_{50} < 500 pM, clear structure-activity relationships were observed; a pharmacophore was developed and used to develop advanced molecular models of the mode of binding. This is the first comprehensive SAR study for inhibitors of these enzymes.

We thank AICR for generous funding.

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2. M. Li, M. D. Threadgill, Y. Wang, L. Cai, X. Lin, Pathobiology 76, 2009, 108.
3. S. J. Hsiao, S. Smith, Biochimie 90, 2007, 83.
4. S. M. A. Huang, Y. M. Mishina, S. Liu, et al. Nature461, 2009, 614.
5. L. Lehtiö, R. Collins, S. van den Berg, et al. J. Mol. Biol. 379, 2008, 136.

Invited Lecturer-1

Dr. Cynthia J. Burrows

Dr. Cynthia J. Burrows is Distinguished Professor of Chemistry at the University of Utah. She was raised in St. Paul, Minnesota and Boulder, Colorado. Her early training was in physical organic chemistry with Prof. Stan Cristol at the University of Colorado (B. A. 1975) and Prof. Barry Carpenter at Cornell University (Ph.D., 1982), followed by a NSF-CNRS postdoctoral fellowship in the laboratory of Prof. Jean-Marie Lehn, Université Louis Pasteur, Strasbourg (1981-83). From 1983-1995, she held the positions of Assistant through Full Professor of Chemistry at the State University of New York at Stony Brook, before returning to the West to take a position at the University of Utah in Salt Lake City in 1995.

Prof. Burrows has been a member of numerous editorial boards and review panels; she currently serves as Senior Editor of the *Journal of Organic Chemistry*. She is a past recipient of the Robert Parry Teaching Award and in 2011 of the University Distinguished Teaching Award; her research was recently recognized with the ACS Utah Award, ACS Cope Scholar Award, and the University of Utah's Distinguished Creative and Scholarly Research Award. In 2009, she was inducted into the American Academy of Arts and Sciences.

IL-1

SINGLE-MOLECULE STUDIES OF OXIDATIVE DAMAGE IN TELOMERIC G QUADRUPLEXES

Cynthia J. Burrows

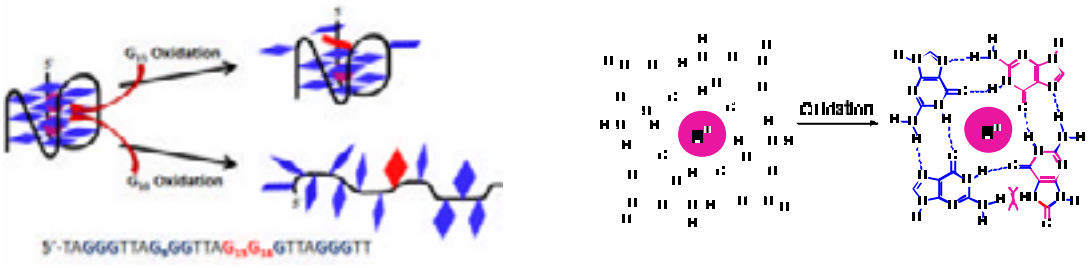
Department of Chemistry, University of Utah, 315 S. 1400 East, Rm 2020, Salt Lake City, Utah 84112-0850, USA.

ABSTRACT

Oxidative damage to the G-rich telomeric sequence at the ends of chromosomes is proposed to be a significant contributor to cellular senescence. In this work, we address several questions related to oxidation of G quadruplexes in synthetic oligomers of the sequence $d(TTAGGG)_n$.

INTRODUCTION

Estimates place the level of DNA oxidative damage to guanine in G-quadruplex sequences as a substantial fraction of the total guanine damage in the genome. Yet, the assessment of guanine oxidation as a function of genome location is complicated by the paucity of methods that provide both sequence information and structural identity of DNA lesions. We recently have taken advantage of a single-molecule technique in which ssDNA is electrophoretically driven through the ? -hemolysin (? -HL) ion channel embedded in a lipid bilayer to analyze the presence of DNA lesions such as 8-oxo-7,8-dihydro-2'-deoxyguanosine (OG) and its further oxidation products (Sp, Gh) as well as for abasic sites (AP).[1-3] This work examined the susceptibility of the 12 guanines of a telomere toward oxidation as a function of the fold (Na^+ vs. K^+), the nature of the oxidant, and the product outcome of the oxidation reactions. In addition, we synthetically incorporated lesions such as OG into specific locations of the telomere (Fig. 1) and monitored the effects on T_m values, CD spectra, and the translocation kinetics of individual strands through the ? -HL nanopore.



RESULTS AND DISCUSSION

In the present work, we find that the location of the G in the sequence and in the layers of the G-quadruplex influence the susceptibility of the G to oxidative damage. For example, one-electron oxidants such as $CO_3^{\bullet-}$ show a strong preference for oxidation of the 5'G of a GGG sequence, and whereas G_9 is a very reactive site when the telomere is folded with K^+, it less reactive in the presence of Na^+ (for sequence, see Fig. 2). In contrast, $^1O_2$ reacts nearly equally at all top and bottom faces of the stacked quadruplexes, but not in the middle layer.

Placement of OG in a top or bottom layer of the telomere results in destabilization and unfolding of that layer, whereas formation of OG in a middle layer leads to complete unfolding of the telomere (Fig. 2). These phenomena could be observed by changes in the T_m values and CD spectra. In addition, we monitored the translocation times of telomeric sequences through the a-HL ion channel and drew correlations between the rates of unfolding and the translocation times. These were highly dependent on the location of lesions in the sequence.

Figure 3. Electrophoretic translocation of DNA through ? -HL.

CONCLUSIONS

The folded form of the telomere influences the reactivity of the various G sites as does the mechanism of oxidation (one-electron vs. singlet oxygen), and the G oxidation products in turn influence the resulting fold. Single-molecule experiments in which damaged DNA strands are threaded through the a-hemolysin nanopore help reveal the kinetics of unfolding of telomeres and may lead to single-molecule sequencing of damage sites.

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1. Schibel, A.E.P., An, N., Jin, Q., Fleming, A.M., Burrows, C.J., White, H.S. *J. Am. Chem. Soc.* **2010**, *132,* 17992-17995.
2. Schibel, A.E.P., Fleming, A.M., Jin, Q., An, N., Liu, J., Blakemore, C.P., White, H.S., Burrows, C.J., *J. Am. Chem. Soc.* **2011**, *133*, 14778–14784.
3. An, N., Fleming, A.M., White, H.S., Burrows, C.J. *Proc. Natl. Acad. Sci.(U.S.A.),* **2012**, *109,* 11504.

Invited Lecturer-2

CV

NAME	POSITION TITLE
Brenton DeBoef	**Associate Professor**

eRA COMMONS USER NAME (credential, e.g., agency login)

bdeboef

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	MM/YY	FIELD OF STUDY
Evangel University	B.S.	05/98	Chemistry, Mathematics
Washington University in St. Louis	A.M.	05/2001	Organic Chemistry
Washington University in St. Louis	Ph.D.	05/2003	Organic Chemistry
Columbia University	Postdoc	06/2005	Organometallic Chemistry

Positions and Employment

Summer 1996	NSF-REU Fellow, University of Arkansas, Fayetteville, Arkansas
Summer 1997	NSF-REU Fellow, Columbia University, New York, New York
Summer 1998	Undergraduate Research Assistant, P&G Pharmaceuticals, Mason, Ohio
1998-2000	Teaching Assistant, Washington University, St. Louis, Missouri
2000-2003	Research Assistant, Washington University, St. Louis, Missouri
2003-2005	Postdoctoral Fellow, Columbia University, New York, New York
2005-2011	Assistant Professor, University of Rhode Island, Kingston, Rhode Island
2011-Present	Associate Professor, University of Rhode Island, Kingston, Rhode Island

Other Experience and Professional Memberships

American Chemical Society (member)

Sigma Xi (faculty sponsor)

Honors

1994-1998	Dean's List, Evangel College (every semester)
1998	Summa Cum Laude, Evangel College
1998	Outstanding Chemistry Graduate, Evangel College
1999	Departmental Award for Teaching Excellence, Washington University
2005	NRSA Postdoctoral Fellowship, NIGMS (declined, so I could accept the position at URI)
2008	Outstanding Young Alumnus, Evangel University
2009	NSF CAREER Award
2011	Pfizer Green Chemistry Award

Service on Governmental Review Panels

2011 & 2013	Reviewer, NSF Panels on Organic Synthesis
2011	Reviewer, NIH Synthetic and Biological Chemistry Study Section (SBCB)

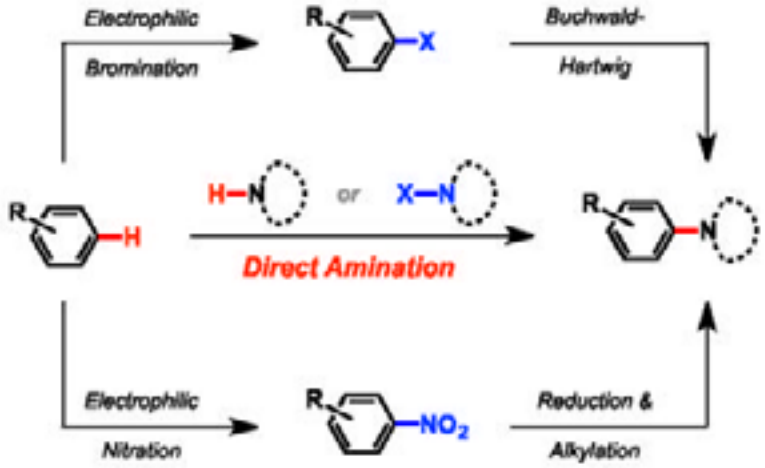
IL-2

Synthesis of C-C and C-N bonds via oxidative C-H functionalization

Brenton DeBoef

Department of Chemistry ,University of Rhode Island ,Kingston,USA

The development of new synthetic methods for cross-coupling via C-H and/or N-H activation would expedite the synthesis of high value target molecules such as biaryls and arylamines by eliminating the pre-functionalization steps that are commonly employed in modern synthetic chemistry. We have recently discovered both metal-catalyzed and metal-free methods for synthesizing both C-C and C-N bonds via oxidative C-H activation. The development of these reactions will be discussed, as well as their application to the synthesis of complex heterocyclic molecules.



Invited Lecturer-3

DR.P.M.S.CHAUHAN, Ph.D, FRSC

M.Sc, 1980, Agra University, Ph**. D** , **1984 , Central Drug Research Institute/** Agra University , Agra

POST DOCTORAL EXPERIENCE AND VISITS ABROAD

Jan 1987 - Oct.1988 (22 months) :**Senior Research Associate** , **Robert Robinson Laboratory, University of Liverpool, UK**

April-2000- July 2000 : Senior DAAD Visiting Scientist, Instituted of Organic Chemistry(RWTH), Aachen, Germany

April 2002 2003, Visiting Scientist, School of Chemical Sciences, **University East Anglia, Norwich,** UK

August 2-9, 2009, Deputation to **Glasgow, UK** (To deliver Key Note,Lecture,42nd IUPAC/RSC, Conference)

Field of Specialization; Synthetic Organic chemistry/Medicinal chemistry,(26 Years), Combinatorial chemistry (11 Years)

Research interests:
Design and synthesis of bio-active heterocycles as Antitubercular, Antimalarial, Antileishmanial and Anticancer agents.

RESEARCH EXPERIENCE AND POSITIONS HELDS

1988 – 2008, Scientist, Central Drug Research Institute , Lucknow
Oct. 2008 - Till date , Scientist-F(Deputy Director), CDRI, ,Lucknow

HIGHLIGHTS OF RESEARCH ACTIVITIES

Paper published in peer reviewed Journals,106,Patents (Indian) Filed; 6
Ph. D. Thesis supervised 11
Total Citaion : 1250Average Citation : 12, H index : 21

Honors and Awards

A. Recipient of the CDRI incentive award for the year 2000.,2001,2010
B. Fellow of Royal Society Chemistry(FRSC) ,2003
C. AWARD for outstanding contributions in Medicinal chemistry and international scientific collaboration (Scientific Partnership Foundation,Moscow,Russia,2005).
D. *Most Cited paper,(**2005-2008**) award by Elsevier* Prem M.S. Chauhan , *Bioorganic and Medicinal Chemistry Letters , 2005, 15*, 531-533
E. Deliver Keynote Lecture, 4^{2nd} IUPAC /RSC Conference on Aug.,2nd -7th 2009 , Glasgow, UK
F. Rashtriya Gaurav Award, 2010, Indian International Friendship Society, New Delhi
G. SEVA CHAKRA PURASKAR,**2011**,by **Exclusive AJTAK** association with All India survey award council

Member: Editorial Board:

H. Editor- in- Chief: Chemistry & Biology Interface
I. Member of Editorial board , Future Medicinal Chemistry,Future science group
J. Member Editorial board , Journal Research and Reports in Medicinal Chemistry
K. Member of Editorial board - Mycobacterial Diseases
L. Member Editorial board ,Global Journal of Organic Chemistry

IL-3

Perspectives and Challenges in Drug Research: Design and Synthesis of Nitrogen Heterocycles as Novel therapeutic Agents

P.M.S.Chauhan

Medicinal and Process Chemistry Division, Central Drug Research Institute Lucknow, India
226001,Email;premsc58@hotmail.com,prem_chauhan_2000@yahoo.com,Phone:91-522-2439492 Fax: +91-522-2623405

Drug research one of the important area of science. It is also very time taking and require multidisciplinary efforts. Nitrogen heterocycles are constituted a major class of existing drugs. These compounds are widely distributed in nature and are essential to life process.They also play a vital role in the controlling the metabolism of all living cells. The activity of these molecules is attributed to their ability to interfere against several imortant biological target sites.

Keeping in view importance of nitrogen hetrocycles in antiparasitic area, we have synthesized novel heterocycles as antiparasitic agents . These heterocycles were synthesized by classical solution phase as well as on solid support. Several synthesized compounds have shown promising *in vitro* and *in vivo* antiparasitic activity against Malaria and Leshimania parasites. The design, synthesis and antiparasitic activity of these **novel therapeutic agents** will be discussed.

Invited Lecturer-4

RACHNA SADANA

Assistant Professor, University of Houston, Downtown, Houston, TX-77002

EDUCATION

1997 – 2001 Ph.D. in Biochemistry, Kurukshetra University, Kurukshetra, India
Dissertation: "Lysosomal Proteolytic Enzymes in Brain"
1994 – 1996 M.S. (Biochemistry), Kurukshetra University, Kurukshetra 136119, India
1990 – 1993 B.S. (Chemistry, Botany and Zoology), S.D. College, Panipat 132103, India

RESEARCH, TRAINING AND PROFESSIONAL EXPERIENCE

Sept 2009 Assistant Professor of Biology and Biochemistry, University of Houston-Downtown (UHD)
June 2010 Adjunct Faculty at University of Texas Health Science center, Medical School, Houston
Spring 2009 Adjunct Faculty at University of Houston-Downtown (UHD)
2004- 2009 Postdoctoral Fellow at University of Texas health Science Center at Houston
2001- 2004 Postdoctoral Fellow at University of Houston-Central Campus
1997- 2001 Ph.D. Dissertation

RESEARCH INTERESTS

- Screening novel compounds to identify novel anti-cancer agents
- Mathematical modeling of kinetics of cAMP formation
- Existence of preformed complexes of adenylyl cyclase and inactive G-proteins

AWARDS AND FELLOWSHIPS

- National Merit Scholarship for High School and College Education
- Gold Medal for M.S. Biochemistry Examination
- University Research Fellowship for Ph.D.: Kurukshetra University (1997-2000)
- Travel Award to Attend JAM-2010 Conference
- Dean's Travel Award to attend ABRCMs 2012

Screening Novel Synthetic Compounds for their Cytotoxicity and Inhibition of Tubulin Polymerization

Rachna Sadana*, Kafayat Busari, and Reyna Valdez

Department of Natural Sciences, 1 Main St., University of Houston-Downtown, Houston, TX-77002, USA

Cancer is a collection of diseases hallmarked by uncontrolled cell division. Cancer treatment involves varying combinations of surgery, radiation, chemotherapy and hormone therapy. Chemotherapy employs the use of drugs that kill the rapidly dividing cells (characteristic of cancer cells). Various chemotherapeutic drugs such as paclitaxel and vinblastine interrupt cell division by binding to tubulin (a protein responsible for spindle formation, a critical step in cell division). For more than 50 years, tubulin binding drugs have been used to treat cancer, Scientists are still in search of novel anti-cancer compounds targeting tubulin for two reasons; (1) patients develop resistance to existing drugs and (2) tubulin is one of the most validated targets for cancer treatment. A series of synthetic thiazoles and coscinamides were evaluated for their cytotoxic effects on 5 different cancer cell lines. Our initial screen using MTT cell proliferation assay identified six compounds that caused cell death with IC_{50} less than 10 μM. The select cytotoxic compounds are currently being investigated for (i) the mechanism of cell death using DNA fragmentation as a marker for apoptotic death and (ii) their ability to interfere with *in vitro* tubulin polymerization using fluorescence based polymerization assay and *in vivo* using immune-fluorescence of tubulin.

Invited Lecturer-5

FERNANDO ALBERICIO

***Address*:**University of Kwazulu-Natal, School of Chemistry,
Westville Campus Phones: 031-2603090Durban 4000, South Africa email: Albericio@ukzn.ac.za

***Personal Data*:**

Birth and Nationality: June 5, 1953. Barcelona (Spain)-Spanish

Marital Status: Widowed. No children.

Education and Training:

University of Barcelona, Department Organic Chemistry, Licenciado 1975,

Master 1976, Ph.D. 1981, Major: Organic ChemistryTufts University, Boston, Department of Protein Chemistry,Research Assistant, 1981Université d'Aix-Marseille, France, Département de Biochimie,

Associate Research Professor (Attaché de Recherche), 1982,University of Minnesota, Department of Chemistry, Research Associate, 1983-1984

***Professional Employment*:**

Barcelona Science Park,Executive Director, 2005-2012,Deputy Director, 1998- 2000

Director for External Relations, 1996-1998.,Millipore Corporation, Boston (USA), Life Science Research Group, Director of,Peptide Research, 1992-1993

DiverDrugs S.L., Barcelona, Spain, Founder, 1999-2007

Medalchemy S.L., Alicante, Spain, Founder, 2001-present

GenMedica S.L., Barcelona, Spain, Founder, 2004-present

Argopharma S.L., Barcelona, Spain, Founder, 2008- present

***Academic Employment*:**

Institut for Research in Biomedicine of Barcelona, Barcelona Science Park

Group Leader, 2003-present,Universitat de Barcelona, Departamento de Química Orgánica,

Professor, 1995-present,Associate Professor, 1985-1995

University of Kwazulu-Natal (Durban, South Africa), School of Chemistry

Research Professor, 2012-present

Awards:

Fourth Leonidas Zervas Award, European Peptide Society, 1994.

Distinction, Research Chair, Generalitat of Catalunya, 2003.

Doctor *Honoris Causa*, Universidad de Buenos Aires (Argentina), 2010.

Vincent du Vigneaud Award, American Peptide Society, 2011.

***Publications*:**

1 Book; 2 Edited Volumes; 618 Papers, Book Chapters, and Minireviews; 47 Patents; 1 Translation

***Other records*:**

43 Ph.D. students; 24 Competitive grants (last 10 years), 13 Industrial contracts (last 10 years)

IL-5

Therapeutic Nanoconjugates

Fernando Albericio, Miriam Royo

[1]Institute for Research in Biomedicine and [2]CIBER-BBN, Networking Centre on Bioengineering, Biomaterials and Nanomedicine, Barcelona Science Park, 08028 Barcelona (Spain); [3]Department of Organic Chemistry, University of Barcelona, 08028 **Barcelona** (Spain); [4]School of Chemistry, University of KwaZulu-Natal, 4041 Durban (South Africa)

As it is well known, the number of new chemical and biological entities being accepted by the Food and Drug Administration is stabilized around 20-30 every year. This relatively low number is due to several factors, but one of the main reasons in the poor ADME properties showed by compounds that previously had been good *in vitro* activity

Invited Lecturer-6

Krishna Nand Singh

Krishna Nand Singh (born in June 1962) obtained his M. Sc. (Organic Chemistry) and Ph. D. (Chemistry) degrees from Banaras Hindu University, Varanasi, India in 1984 and 1991 respectively. After a short post-doctoral tenure, he joined the Department of Applied Chemistry, Banaras Hindu University as Assistant Professor in 1993, where he was elevated to the post of Associate Professor in 2002. He moved to the Department of Chemistry, Banaras Hindu University as Full Professor of Organic Chemistry in the year 2007. He has received eleven major research projects as Principal Investigator from different agencies and also been an Invited Professor, CNRS, University of Rennes, France (2004).

His current research interests include green chemistry, microwave assisted organic synthesis, multi-component reactions, and transition metal catalyzed organic reactions. Altogether seven students have awarded Ph. D. degrees under his supervision and eight are working at present. His research work has resulted in the publication of seventy eight publications in reputed journals.

Development of Some Green Protocols for Organic Synthesis

Krishna Nand Singh

Professor of Organic Chemistry
Department of Chemistry, Faculty of Science, Banaras Hindu University, Varanasi-221005, India
E-mail: knsinghbhu@yahoo.co.in; knsingh@bhu.ac.in

In today's world, synthetic chemists in both academia and industry are constantly challenged to think about more environmentally benign methods for generation of the desired target molecules. As a result, green chemistry has presently attained the status of a major scientific discipline. The investigation and application of green chemistry principles has led to the development of cleaner and more benign chemical processes, with many new technologies being developed each year. Microwave has emerged as a novel and benign source of energy for chemical reactions and has been extensively investigated in organic synthesis during recent years. Compared to conventional thermal heating, the use of microwave provides chemical processes with special attributes, such as enhanced reaction rates, higher yields, enhanced product purity, better selectivity, ease of manipulation, rapid optimization of reactions and several eco-friendly advantages.

Catalyst and solvent usage is often an integral part of a chemical or manufacturing process. The unavoidable choice of a specific catalyst or solvent for a desired chemical reaction can have profound economical, environmental, and societal

implications. The pressing need to develop alternative reaction conditions originates from these implications and constitutes an essential strategy under the emerging field of green chemistry. Toward this end, considerable efforts have been devoted to develop and use nontraditional catalysts and solvents for chemical synthesis.

In view of the above and as a part of our ongoing research interest, some recent results on the development of green protocols in organic synthesis will be discussed.

[1]. D. S. Raghuvanshi, A. K. Gupta, and Krishna Nand Singh, *Organic Letters*, 14 (2012) 4326.

[2]. N. Singh and Krishna Nand Singh, *SYNLETT*, 23 (2012) 2116.

[3]. K. Kumari, D S Raghuvanshi and Krishna Nand Singh, *OPPI*, 44 (2012) 460.

[4]. A. K. Gupta, Tirumaleswara Rao G. and Krishna Nand Singh *Tetrahedron Letters*, 53 (2012) 2218.

Invited Lecturer-7

Chemical biology of GPI molecules

Ram Vishwakarma

Indian Institute of Integrative Medicine, Jammu,

Invited Lecturer-8

Steven E. Rokita, Brief Curriculum Vitae

Department of Chemistry, Johns Hopkins University, 3400 N. Charles St., Baltimore, MD 21218, USA
Tel: +1-410-516-5793, fax: +1-419-516-8420; Email: rokita@jhu.edu

1. Current Appointment

2012 Professor of Chemistry, Johns Hopkins University, Baltimore, MD

2. Education

1979 B.S. Chemistry, College of Chemistry, Univ. of California, Berkeley, CA

1983 Ph.D. Biological Chemistry, Dept. of Chemistry, MIT, Cambridge, MA

1983-85 NIH post-doctoral Fellow, Rockefeller University, NY, NY

3. Career Development

1986-95 *Assistant & Associate Professor* of Chemistry, University at Stony Brook

1995-2012 *Associate & Full Professor* of Chem. & Biochem., Univ. of Maryland

4. Awards/Honors/Fellowships

1998 Catacosinos Young Investigator in Cancer Research (SUNY Stony Brook)

1999 Chair, Bioorganic Gordon Research Conference

2001 Outstanding Invention of 2001, (Novel Copper Compexes, Univ. of MD)

2005 Faculty Excellence Award in Research, College of Life Sci. (Univ. of MD)

2006 Faculty Excellence in Service, College of Life Sci. (Univ. of MD)

2009 Honorary Fellow of the Indian Society of Chemists and Biologists

2011 Fellow, American Association for the Advancement of Science (AAAS)

2011 Editorial Advisory Board of *Chemistry & Biology Interface*

2012 Chair, Enzymes, Coenzymes and Metabolic Pathways Gordon Conference

5. Research Interests

Sequence and conformation specific reactions of nucleic acids; enzyme-mediated activation of substrates and coenzymes; halogenation and dehalogenation reactions in biology; aromatic substitution and quinone methide generation in bioorganic chemistry; copper- and nickel-mediated reactions in bioinorganic chemistry, electron transfer in biopolymers

6. Selected Publications (total 97)

Huan Wang and Steven E. Rokita "Dynamic Cross-linking is Retained in Duplex DNA After Multiple Exchange of Strands" *Angew. Chem. Int. Ed.* **2010**, 49, 5957-5960.

Clifford S. Rossiter, Emilia Modica, Dalip Kumar, and Steven E. Rokita "Few Constraints Limit the Design of Quinone Methide-Oligonucleotide Self-Adducts for Directing DNA Alkylation", *Chem. Commun.* **2011**, *47*, 1476-1478.

Abulfazl Fakhari M. and Steven E. Rokita "A New Solvatochromic Fluorophore With High Sensitivity for Studying Biopolymers" *Chem. Commun.* **2011***, 47,* 4222 - 4224.

Michael P. McCrane, Emily E. Weinert, Ying Lin, Eugene P. Mazzola, Yiu-Fai Lam, Peter F. Scholl, and Steven E. Rokita "Trapping a Labile Adduct Formed between an *ortho*-Quinone Methide and 2'-Deoxycytidine" *Org. Lett.* **2011**, *13*, 1186–1189.

Yang Liu and Steven E. Rokita "Inducible Alkylation of DNA by a Quinone Methide-Peptide Nucleic Acid Conjugate" *Biochemistry* **2012**, *51*, 1020-1027.

Editor, *Quinone Methides* as Vol. 1 of the *Wiley Series on Reactive Intermediates in Chemistry and Biology*. Wiley: Hoboken, 2009, pp. 431. [ISBN: 978-0-470-19224-5]

Serial Editor and Founder of *Wiley Series on Reactive Intermediates in Chemistry and Biology*.

IL-8

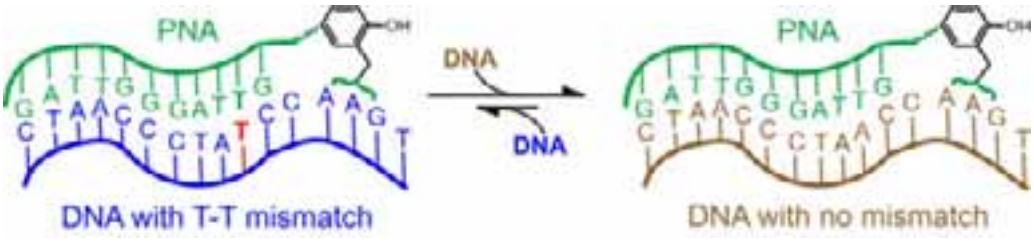
DYNAMIC AND TARGETED ALKYLATION OF DNA

Steven E. Rokita

Department of Chemistry
Johns Hopkins University, 3400 N. Charles St., Baltimore, MD 21218, USA.
Rokita@jhu.edu

Methods for controlling the specificity of covalent reagents in biomimetic and biological systems continue to challenge chemists and biochemists since the goals of "fast acting" and "highly selective" are often mutually exclusive. To date, poor specificity has been tolerated for anticancer treatments based on irreversible alkylation of DNA since few practical alternatives are yet available. Strategies based on non-covalent interactions may offer the potential of improved specificity, but their DNA•drug complexes would rapidly dissociate when the helical structure of DNA becomes denatured by enzymes responsible for replication and transcription. Reversible alkylation represents an attractive compromise for optimizing selectivity and biological efficacy. This approach should generated DNA adducts of sufficient persistence for preventing expression of a chosen gene and yet maintain the necessary dynamics for reversing off-target reactions that would otherwise consume reagent and cause collateral damage to cells. Model studies based on the reactions of a simple electrophilic *ortho*-quinone methide (QM) and nucleosides revealed high yields of kinetics products along with the expected products of greatest thermodynamic stability.[1] Concurrently, the dynamics of QM regeneration from the kinetic products were detected over hours and

determined to be very sensitive to electron withdrawing and donating substituents. Covalent cross-linking by derivatives supporting tandem formation of two QM intermediates (bisQM) was similarly reversible and remained active over many days as observed through strand exchange studies.[2] Reversibility has also been demonstrated with oligonucleotide-QM conjugates that were designed to carry their electrophilic intermediate to selected targets through formation of self-adducts. Intramolecular reaction and interstrand transfer of the QM is very rapid and remains competitive even in the presence of high concentrations of strong nucleophiles such as 2-mercaptoethanol. The ability to form reversible self-adducts and direct alkylation to selected targets has recently been extended to a wide range of nucleotide sequences.[3] Thymine remains unreactive to QM, but adenine, cytosine or guanine reversibly trap and release QM. Even sequences containing only a few cytosines embedded in a thymine-based oligonucleotide are sufficient to support reversible target alkylation. This result was prerequisite for deliverying a QM to duplex DNA using triplex recognition. In anticipation of cellular studies, sequence-directing oligonucleotides have been replaced with peptide nucleic acids (PNA) that associate strongly to their DNA targets but are neutral and biologically stable.[4] These conjugates provide a very high level of discrimination between fully complementary and mismatch-containing targets.



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1. S. E. Rokita. In *Quinone Methides*. (ed. S.E. Rokita), pp. 297-327. Wiley: Hoboken, 2009.

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Invited Lecturer-9

Mahesh K. Lakshman, Ph.D.

The City College and The City University of New York, Department of Chemistry
160 Convent Avenue, New York, NY 10031

Education

Ph.D.	(Organic Chemistry)	University of Oklahoma	July 1989 (GPA 3.9/4.0)
M.S.	(Organic Chemistry)	University of Oklahoma	December 1987
M.Sc.	(Organic Chemistry)	University of Bombay	May 1984
B.Sc.	(Chemistry)	University of Bombay	May 1982

Appointments

- **The City College and The City University of New York, New York, NY**
  - *Executive Officer (Chair Equivalent, City University of New York PhD program in Chemistry)* July 2008–June 2011
  - *Professor of Chemistry* September 2008–present
  - *Associate Professor of Chemistry* January 2004–September 2008 (early tenure)
  - *Assistant Professor of Chemistry* August 2000–Dec 2003
- **University of North Dakota, Grand Forks, ND** *Assistant Professor* January 1998–August 2000
- **Chemsyn Science Laboratories, Lenexa, KS** *Senior Scientist* August 1994–December 1997
- **National Institutes of Health, Bethesda, MD** *Fogarty Fellow* December 1989–August 1994

Awards and Merits

2011	The City College of New York President's S.T.A.R (service, teamwork, action, and results) Award
2011	*Excellent service to the Editors and Authors of EurJOC European Journal of Organic Chemistry*, Certificate of Recognition from Wiley-VCH and ChemPubSoc, Europe
2007	*In honor of Outstanding Scholarly Achievements and Contributions to the Creation and Transmittal of Knowledge*, Certificate of Recognition from The City University of New York
2007	*Certificate of Appreciation* from the Alfred P. Sloan Foundation for commitment to advancing underrepresented minority students in mathematics, science and engineering and for partnering with the Foundation's Minority Ph.D. Program.
2007	Profiled in the June 1 issue of *India Abroad* (page A28, paper has US circulation).
2006	*For Securing Major Institutional Grant Funds in 2005*, Certificate of Recognition from The City University of New York
2004	*In honor of Outstanding Scholarly Achievements and Contributions to the Creation and Transmittal of Knowledge*, Certificate of Recognition from The City University of New York
2003–2004	*Outstanding Mentor Award* The City College of New York
2003	*Recipients of Major Institutional Grants for Public Service*, Certificate of Recognition from The City University of New York
2001 & 2002	*In honor of Outstanding Scholarly Achievements and Contributions to the Creation and Transmittal of Knowledge*, Certificate of Recognition from The City University of New York
1989–1994	*Fogarty Fellow*, National Institutes of Health
1988–1989	*Dow Fellow*, University of Oklahoma
1988	*Cleo Cross International Student Fellow*, University of Oklahoma (1 of 13 students selected from all departments)
1986	*Teaching Excellence Award*, University of Oklahoma

Professional Service

- Co-chair, lecture session at Frontiers in Pharmaceutical Sciences: Global Perspectives (International Conference), University of Rhode Island, September 28–30, 2012.
- Co-chair oral presentation session at 14th ISCB International Conference, Lucknow, India, January 2010
- Editorial Board member of *Organic Chemistry International*, 2008–present
- Editorial Board member of *Current Chemical Biology*, 2007–present
- Editorial Board member of *Acta Chimica Slovenica*, 2005–present
- Member *National Institutes of Health* Study Section ZRG1 F04A-L 20L, Oct 2008.
- Panelist *National Science Foundation* Organic and Macromolecular Chemistry, Mar 2008.
- Panelist *National Science Foundation* Major Research Instrumentation, May 2006.
- Member *National Institutes of Health* SBIR/STTR Study Section ZRG1 ONC-T 10B, 2005–2007.
- Chemistry Panelist: PSC-CUNY grant application review panel, 2001–2009.
- *Ad hoc* proposal reviewer for the *National Science Foundation* and *American Chemical Society PRF Grants* and *Research Corporation*.
- On-site presentation judge: Annual Biomedical Research Conference for Minority Students (ABRCMS), New Orleans, Louisiana, 2002.

IL-9

N-Directed C–H Bond Activation in Purines and Purine Nucleosides

Mahesh K. Lakshman

Professor, Department of Chemistry

The City College and The City University of New York, 160 Convent Avenue, New York, NY 10031

Metal-catalyzed C–H bond activation provides a versatile and highly attractive synthetic approach for the functionalization of diverse organic molecules. Among the various heteroatom directing groups, nitrogen atom stands out as a major C–H bond activation director. Nucleosides are ubiquitous in nature and nucleoside modification is a highly significant aspect of biomolecular functionalization. Purines contain four nitrogen atoms, in addition purine nucleosides contain oxygen atoms and a labile glycosidic bond. This renders C–H bond activation chemistry of purines and purine nucleosides a non-trivial problem. Nevertheless, under appropriate conditions C–H bond activation of purines and purine nucleosides can be conducted with ruthenium and palladium catalysts, leading to complex functionalization of these biomolecules.

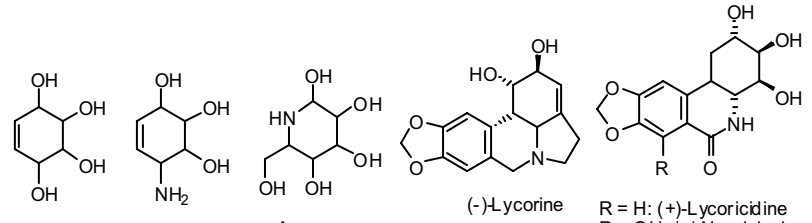
Invited Lecturer-10

Stereoselective Synthesis of Aminocytitols by Using Carbohydrate Based Building Blocks: Formal Synthesis of (+)-Conduramine E and (-)-Conduramine E

Arun K. Shaw

Division of Process and Medicinal Chemistry, CSIR-Central Drug Research Institute, Chattar Manzil, M. G. Marg, Lucknow
Email: akshaw55@yahoo.com

Aminocyclohexenetriols formally known as conduramines are the amino derivatives of conduritols, in which one of the hydroxyl groups is replaced by an amino functionality (Figure 1). These highly functionalized aminocyclohexenetriols and structurally related compounds form the basic skeleton of several complex aminoglycoside antibiotics and pseudo oligosaccharides.[1-3] They are also the precursors for the synthesis of pharmacologically important molecules with important bioactivities like antibacterial, antihypertensive, platelet-inhibiting, cytotoxic (Figure 1).[4-6] The stereoselective route for the synthesis of aminocytitols from carbohydrates was recently achieved in our laboratory. The formal synthesis of (+)-conduramine E and (-)-conduramine E was successfully completed by utilizing this strategy.[7] One pot three component Petasis-Borono-Mannich reaction to introduce the *syn*-ß-amino alcohol functionality of conduramine E and ring closing metathesis to construct its carbocyclic core were the key features of the synthetic strategy. The present synthetic approach paves the way for stereoselective synthesis of several conduramines starting from carbohydrates.



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Invited Lecturer-11

Ashok K Prasad

Professor, Department of Chemistry, University of Delhi, *Delhi- 110 007*
Email: ashokenzyme@yahoo.com

Professor Ashok Prasad obtained his PhD from University of Delhi in 1990.**Postdoctoral positions** at the University of Southern Denmark, Odense and University of Copenhagen, Denmark; **Visiting researcher** at Max-Planck-Institute for Molecular Physiology, Dortmund, Germany; UMASS, Lowell, USA, CNR Laboratories, Italy, etc.**Major research interests** include synthesis of modified nucleosides and oligonucleotides involving them and efficient methodology development using lipases as selective biocatalysts. **Recipient of** DANIDA Fellow (1992-96), CRSI Young Scientist Award 2007, Visiting Associate Professorship, Department of Physics and Chemistry, University of Southern Denmark, Denmark (July 2009-June 2010), Best Paper Award- 2012 of the journal *Trends in Carbohydrate Research*, etc.**Has been the Guest editor** *Biochemie*, a journal published by Elsevier (Impact Factor ~4) and *Indian J. Chemistry*, Section B.**PUBLICATIONS: 160 Research Papers** in the International Journal of Repute

PATENTS: 10 International and Indian Patents in his credit

Total Citations of his Publications: 1550

***h* Index** of his publications: **20**

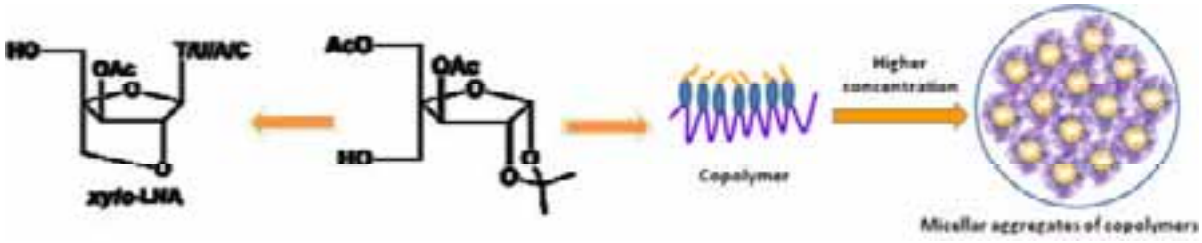
From Glucose to Modified Nucleosides, pH Sensitive Sugar-based Polymers and Crown Ethers of Importance

Ashok K. Prasad

Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi-110 007
E-mail: ashokenzyme@yahoo.com

The discovery of sugar modified nucleoside derivatives as potential antiviral agents and the emergence of antisense and antigene oligonucleotides as potential and selective inhibitors of gene expression have led to the considerable rise in the synthesis of modified nucleoside derivatives and nucleic acids involving them. Further, there has always been need to have biocompatible drug carriers capable of delivering water insoluble drugs with high transport and controlled release capacity.

We have developed an efficient biocatalytic methodology for the transformation of a trihydroxy sugar derivative derived from glucose into *xylo*-LNA, a monomer of antisense oligonucleotide and sugar-PEG co-polymer having application as drug carrier and its controlled release. Detailed results will be presented in the meeting.



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Invited Lecturer-12

Donal F. O'Shea, Ph.D.

Centre for Synthesis and Chemical Biology
School of Chemistry and Chemical Biology, University College Dublin, Ireland
Tel: 353-(0)1-7162425 e-mail: donal.f.oshea@ucd.ie; http://www.ucd.ie/chem/staff/profdonaloshea/

Employment and Educational Background

2007 - to date:
Associate Professor, Head of Organic Chemistry Section, School of Chemistry and Chemical Biology, University College Dublin, Dublin.

2005 - 2007:
Senior Lecturer, School of Chemistry and Chemical Biology, University College Dublin.

2002 - 2003:
Co-Director of the Centre for Synthesis and Chemical Biology, University College Dublin.

1999 - 2004:
College Lecturer, Department of Chemistry, University College Dublin.

1997 - 1999:
Research Scientist; Color Technology Research Division, Eastman Kodak Company, Rochester, New York, USA.

1996 - 1997: (Research group of Prof. Jon Lindsey)
Postdoctoral Research Fellow; North Carolina State University, Raleigh, NC, USA.

1995 - 1996: (Research group of Prof. Jon Lindsey)
Postdoctoral Research Fellow; Carnegie Mellon University, Pittsburgh, PA, USA.

1993 - 1995: (Research group of Dr. John Sharp, (retired))
Postdoctoral Research Fellow; University of Edinburgh, UK.

1990 - 1993:
Ph.D. University College, Galway.

1986 - 1990:
B.Sc. University College, Galway, Ireland.

Research Group

Current Research Group:
Research group currently consists of five Ph.D. students and four postdoctoral researchers.

Students Graduated:
Nine Ph.D. and three M.Sc. students graduated to date.

Postdoctoral Researchers:
Supervised sixteen post-doctoral researchers.

Erasmus Students:
Supervised fifteen international visiting students.

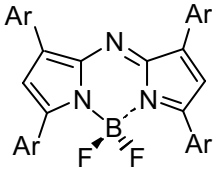
IL-12

BF_2-Azadipyrromethene Based *in vivo* Near Infrared Fluorescence Imaging Platforms

Donal O'Shea

School of Chemistry and Chemical Biology,University College Dublin,Ireland, Email:donal.f.oshea@ucd.ie

We have recently developed the BF_2-chelated azadipyrromethenes **1** as a new class of near-IR fluorophore with medicinal and imaging applications. Fluorescence imaging, utilizing molecular fluorophores, often acts as a central tool for the investigation of fundamental biological processes and offers huge future potential for human imaging coupled to therapeutic procedures. An often encountered limitation with fluorescence imaging is the difficulty in discriminating non-specific background fluorophore emission from fluorophore localized at a specific region of interest. This limits imaging to individual time points at which background fluorescence has been minimized. It would be of significant advantage if the fluorescence output could be modulated from *off* to *on* in response to specific biological events as this would permit imaging of such events in real time without background interference. Here we report our approaches to achieve this for the most fundamental of cellular processes i.e. endocytosis. We describe near-infrared *off* to *on* fluorescence switchable molecular and nanoparticle based constructs that are capable of switching fluorescence on following cellular uptake but remain switched off in extracellular environments. This permits continuous real-time imaging of the uptake process as extracellular particles are non-fluorescent. The principles behind the cellular controlled fluorescence off/on switches will be outlined.



1

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Invited Lecturer-13

Athina Geronikaki

1971 - Graduated from Tashkent State University and gained the speciality of organic chemist

1971 - 1977 - A post-graduate student and researcher at the Institute of Chemistry of Natural Products of Uzbek Academy of Science.

1977 - I defended the Thesis and received the Ph.D grade in chemistry.

1978 - Ph.D. , Doctor of Philosophy in Chemistry.

1984 - Graduated from Aris totelian University of Thessaloniki and gained the speciality of pharmasist

Scientific interest

Chemistry of natural products - isolation, determination of structure.

Chemistry of biologically active compounds and evaluation of their activity

Organized 2 International conferences: Computational Methods in Toxicology and Pharmacology, Integrating Internet Resources (2003) Thessaloniki; 4th Eurasian Meeting on heterocyclic Chemistry , 2006 , Thessaloniki

Member of organizing committee of more than 20 confe rences

Internationa editor in journal Revista de Ciências Farmacêuticas Básica e Aplicada/ Journal of Basic and Applied Pharmaceutical Sciences and

Member of Advisory Board of Jordan Journal of Chemistry

ARTICLES more than 70 (76)

Announcement in International Conferences 135

Books 4 (for students) .

Awarded with medal for development of International collaboration by the Scientific Partnership Foundation,

Awarded with Diplom for the investment in development of science and of international collaboration by the Scientific Partnership Foundation.

DESIGN AND SYNTHESIS OF NOVEL (4/6-SUBSTITUTED BENZO[d] THIAZOL-2-YL)THIAZOLIDINONE-4-ONES WITH ANTIMICROBIAL ACTIVITY

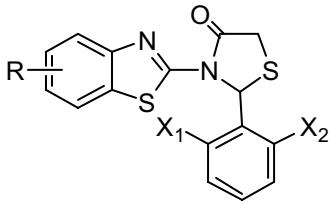
Pitta E.[1], Geronikaki A.[1], Glamoclija J.[2], Ciric A.[2], Sokovic M.[2]

[1]School of Pharmacy, Dep/t Pharm. Chemistry, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece
[2] Institute for Bio logical Research "S. Stankovic", Bul. Despota Steafana 142, Belgrade, Serbia
E-mail: geronik@pharm.auth,gr

Through the past decades, the rapid progress of science had undoubtedly as a result, the significant progress in the diagnosis and treatment of infectious diseases. Despite these efforts, the emerging resistance of microorganisms to known antibiotics kept the scientific interest high, in developing new classes of antimicrobial compounds. In addition, the need for effective

antimicrobial drugs became even greater considering the difficulties of dealing with the treatment of infected hospitalized patients and protection of immunosuppressed and HIV-infected patients.

Therefore, designing innovating drugs with different mode of action could be the choice of preference in order to overcome the problem of cross resistance to existing therapeutics Thus, in our design we emphasize on the strategy of combining two chemically different but pharmacologically compatible molecules, the thiazolidin-4-one nucleus and the benzothiazole group in one frame. Benzothiazolyl/thiazolidinone derivatives with various biological activities have been synthesized by many investigators during the last decades. Analgestic, anti-inflammatory, COX, LOX inhibitory action and antimicrobial activity are among the pharmaceutically interesting properties that were detected in different benzothiazolyl/thiazolidinone derivatives during the past years. Taking into account the interesting properties of these derivatives and in continuation of our research, we designed and synthesized a series of novel 2-aryl-3-benzo[d]thiazol-2-yl-1,3-thiazolidin-4-ones (Scheme 1).



Scheme1.

In order to investigate their antimicrobial (MIC, MBC) and antifungal activity (MIC, MFC), all newly synthesized compounds were tested against a panel of human pathogenic bacterial and fungi, using the microdilution method.

As reference drugs were used a) ampicillin, streptomycin and b) ketoconazole, bifonazole for the antibacterial and antifungal assays respectively.

Invited Lecturer-14

A Preeminent Combination of Approach and Technology: Green nanotechnology towards Sustainability

Anshu Dandia

Centre of Advanced Studies, Department of Chemistry, University of Rajasthan, Jaipur-302004 India
E-mail: dranshudandia@yahoo.co.in

The biological activity and structural complexity found in nature has stimulated generations of synthetic chemists to design strategies for assembling challenging structures found in natural products. Further, in view of ever increasing demand for novel medicinally active compounds, the most important goal for chemists is to ensure that the next generation of synthetic protocols for drugs and fine chemical synthesis is more sustainable and greener than the current generation. For this "green nano" combination is decisive for addressing both economic and environmental issues.

Recently, there has been growing interest in using nanoparticles in organic synthesis and these are foreseen as an active area of research in the future. Thus, we modified the laborious process of lead discovery by accumulating green methodologies and nanotechnology in combination with aqueous media to result in synthesis of a wide variety of novel spiro heterocycles (Dandia et al. [1]) and biologically important scaffolds via facile tandem reactions using non-conventional energy sources, e.g., ultrasound and infrared radiation, which dramatically reduced chemical waste and reaction times along with increased selectivity of the process. Besides, the nanocatalysts were found to possess more potent catalytic activity, easy preparation, high stability, ease of recyclability as well as proved greener compared to traditional catalysts.

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Invited Lecturer-15

Antimalarial Drug Development: From Simple in vitro Screening to Lead Identification

Diwan S Rawat*

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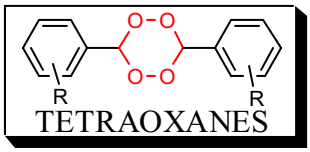
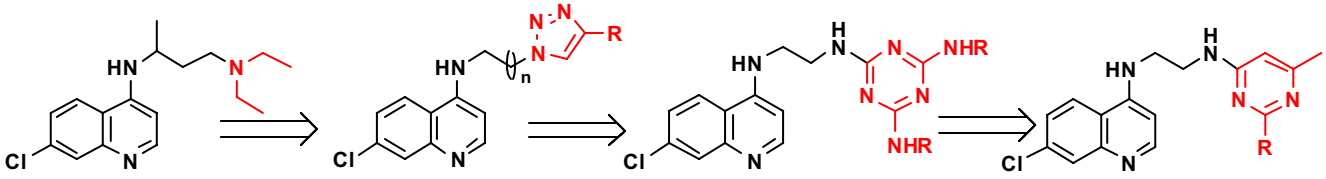
Malaria is still one of the deadly diseases causing deaths of more than 0.7 – 1 million people per year all over the world. Amino-quinolines have been used for the treatment of malaria for a long time, but *Plasmodium falciparum* has developed resistance against these compounds, and artemisinin and its derivatives are the only alternative for the treatment of *Plasmodium falciparum* related infections [1,2]. Heme and dihydrofolate reductase are the most commonly studied targets in malaria chemotherapy [3,4]. Aminoquinoline and artemisinin based compounds stop the hemozoin formation *via* different mechanism, while cycloguanil, a triazine derivative exhibit antimalarial activity due to its ability to inhibit dihydrofolate reductase enzyme. Recently another class of compound named tetraoxanes received considerable amount of interest due to it artemisinin like activity, however, the structural diversity of this important class of compounds is not available [5,6]. To this end, synthesis, characterization, x-ray crystal structure, antimalarial activity and cytotoxicity of symmetrically and asymmetrically substituted tetraoxanes, tetraoxane based hybrids, and novel aminoquinoline conjugates will be presented [7-17].





IC_{50} = 0.048 (D6) µM
IC_{50} = 0.43 (W2) µM

IC_{50} = 0.92 (D6) µM
IC_{50} = 1.37 (W2) µM

IC_{50} = 0.07 (D6) µM
IC_{50} = 0.71 (W2) µM

IC_{50} = 0.007 (D6) µM
IC_{50} = 0.016 (W2) µM
Better than chloroquine (*in vitro* and *in vivo*)

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Invited Lecturer-16

Chiral Catalysis an Important Tool for the Synthesis of Pharmaceutically Active Molecules

R.I. Kureshy*

*Discipline of Inorganic Materials and Catalysis, Central Salt and Marine Chemicals Research Institute (CSMCRI), Council of Scientific & Industrial Research (CSIR), G. B. Marg, Bhavnagar- 364 002, Gujarat, India.E-mail: mailto:khan251293@yahoo.in rukhsana93@yahoo.co.in

ABSTRACT

Increasing demand of chiral compounds in pharmaceuticals has made the role of asymmetric catalysis very important because one enantiomer of a chiral drug molecule is likely to show desirable therapeutic effects while other enantiomer can have a different or adverse biological response. In order to differentiate these contradictory effects, the biological activity of each enantiomer needs to be studied separately. Among the various strategies to develop the desired enantio-pure product, catalytic asymmetric synthesisis the most economic way to produce thousandof chiral compounds by the use of a small amount of chiral catalyst.This field has contributed significantly towards the requirement of enantiomerically pure compounds particularly in pharmaceutical industry via designing of efficient chiral catalysts. Our efforts in designing of chiral metal complexes for the synthesis of enantio-pure products as key intermediate for pharmaceuticals will be presented.

Invited Lecturer-17

Maria Laura Bolognesi

Place and Date of Birth: Teramo (Italy) – September 23, 1966;

Education

Degree in Pharmaceutical Chemistry and Technology, 1990, University of Bologna

Degree in Pharmacy, 1992, University of Bologna

Ph.D. in Pharmaceutical Sciences, 1996, University of Bologna

Professional Experience:

Researcher at the Chemistry Department, 1991-1992, Sigma Tau, Rome

Research fellow, 1994, Dept of Medicinal Chemistry, University of Minnesota

Post-doctoral fellow, 1996-1998, Dept of Pharmaceutical Sciences, University of Bologna

Assistant Professor of Medicinal Chemistry, 1998-2005, University of Bologna

Associate Professor of Medicinal Chemistry, 2005-present, University of Bologna

Research Interests:

Design and synthesis of small molecules as probes for the investigation of biological processes or as drug candidates for neurodegenerative and neglected tropical diseases. In particular, she is currently focusing her research efforts on the identification of multitarget ligands as innovative therapeutic tools. All these activities have resulted in the publication of more than 85 original papers in international journals with a high impact factor (*Angew. Chem. Int. Ed. Engl.* (1), *Med. Res. Rev.* (1), *Curr. Opin. Chem. Biol* (1)., *J. Med. Chem.*(31), *Neurotherapeutics* (1) etc), 4 book

chapters (edited by Royal Society of Chemistry, Wiley, Elsevier), 4 international patents, and in the delivery of more than 25 invited lectures and seminars.

Honors:

1991 "A. Pistani" Lions Award, as the best student from the Faculty of Pharmacy.

1991 "L. Pesci" Award for the best thesis in Medicinal Chemistry.

2003 and 2004 University Award for teaching excellence.

2009 Programa de visitantes distinguidos (Distinguished Visiting Professor), Universidad Complutense Madrid (Grupo Santander)

Professional Services

2006-Present: Coordination of an Erasmus/Socrates exchange program with the Universidad Complutense of Madrid**.**

2007-2009: member of the Faculty for the Doctoral course on Physics and Chemistry of Biological Systems (Curriculum in Drug Discovery) at the International School for Advanced Studies (SISSA) of Trieste.

2010-Present: member of the Faculty for the Doctoral Course on Drug Discovery (School of Life and Humanoid Technologies) at the Italian Institute of Technology (IIT)/University of Genoa.

2011-Present member of the Faculty for the PhD Course in Structural and Functional Genomics at the International School for Advanced Studies of Trieste.

2010: Session Organizer, *Polypharmacology: Creating Selective Non-Selectivity*, in: Trekking through Receptor Chemistry, 28th Camerino-Cyprus-Noordwijkerhout Symposium, (Camerino, Italy)

2012: Scientific Committee, European School of Medicinal Chemistry

2012: Local Organizing Committee 6° Meeting "Nuove Prospettive in Chimica Farmaceutica" (Riccione, Italy)

Editorial, Refereeing and Reviewing Activities:

In the Editorial Board of ChemMedChem, Current Medicinal Chemistry, Current Topics in Medicinal Chemistry (CNS Editor) and Current Chemical Biology.

Designing multitarget drugs for neurodegenerative diseases

Maria Laura Bolognesi

Alma Mater Studiorum-Università degli Studi di Bologna, Dipartimento di Farmacia e Biotecnologie, Bologna, Italy, marialaura.bolognesi@unibo.it

Despite the large research effort, for Alzheimer's and other neurodegenerative disease there is no cure. The molecular mechanisms of these diseases involve a complex array of processes operating simultaneously and synergistically, including: (i) protein aggregation; (ii) oxidative stress; (iii) mitochondrial dysfunction; (iv) unbalance of metal ions. Therefore, it is extremely challenging to develop therapies for major neurodegenerative diseases. The dominant drug discovery paradigm is 'one disease, one target, one molecule', which ignores the polyetiological nature of such maladies. Thus, this paradigm has been shown to be a possible factor in the ongoing failure of current neurotherapeutic drugs. An alternative approach involves single chemical entities that interact simultaneously with multiple targets, the so-called multitarget drugs. This polypharmacological approach is more promising because it is more adequate at addressing the multifactorial and progressive pathophysiological processes involved in neurodegeneration.

By way of illustration of this principle, in this lecture, using examples taken from my own research, I will propose MTDs as innovative tools for addressing the drawbacks and pitfalls of current drug discovery.

Invited Lecturer-18

Tsann-Long Su, Ph.D.

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Date of Birth: March 29, 1945.
Place of Birth: Hsinchu, Taiwan.
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Tel: +886-2-2789 9045 **Fax**: +886-2-2782 9142, +886-2-2782 7685
e-mail: tlsu@ibms.sinica.edu.tw

Education:

1969, B.S.,	School of Pharmacy, Kaohsiung Medical College, Taiwan
1977, Ph.D.	Medicinal Chemistry, Free University of Berlin, Berlin, Germany

Postdoctoral Training:

1977-1978	Postdoctoral Researcher, Schering AG, Berlin, Germany

Position and Appointments:

1970-1974	Teaching Assistant, Kaohsiung Medical College, Taiwan
1979-1980	Associate Researcher, Laboratory of Organic Chemistry, Memorial Sloan-Kettering Cancer Center (MSKCC), NY, USA
1981-1995	Associate Laboratory Member, MSKCC, NY
1995/8-present	Research Fellow, Institute of Biomedical Sciences (IBMS), Academia Sinica, Taipei, Taiwan
1997-1999	Deputy Director and Research Fellow, IBMS, Academia Sinica

Research Description

1. Design and synthesis of DNA-directed alkylating agents and bi-functional alkylating agents.
2. Design and synthesis of potential DNA topoisomerases I and II mediated anticancer agents.
3. Discovery and development of antitumor natural products with novel mechanism of action.

Publications

Total 96 publications and 16 US patents.

Novel antitumor indolizino[6,7-*b*]indoles with multiple modes of action: DNA cross-linking and topoisomerase I and II inhibition

Tsann-Long Su

Institute of Biomedical Sciences, Academia Sinica, Taipei 11529, Taiwan, tlsu@ibms.sinica.edu.tw

DNA bifunctional cross-linking agents are wildly used as chemotherapeutic agents in clinics for the treatment of cancers. These agents possess two reactively electrophilic centers, which are capable of interacting with DNA to form interstrand or intrastrand cross-linking and inducing a number of different lesions. Among DNA cross-linking agents, Mitomycin C (MMC) and pyrrolizidine alkaloids bear a pyrrolizine moiety, which contains two reactive centers to bind covalently with DNA double-strands. Recently, we have synthesized a series of bis(hydroxymethyl)indolizino[6,7-*b*]indoles and their bis(alkylcarbamate) derivativesd for antitumor studies. These agents were designed as hybrid molecules of ß-carboline (topoisomerase inhibition moiety) and bis(hydroxymethyl)pyrrole (DNA cross-linking moiety). The preliminary antitumor studies indicated that these agents exhibited significant antitumor activity in the growth inhibition of a variety of human tumor cells in vitro. Treatment of human breast carcinoma MX-1 xenograft-bearing nude mice with compounds BO-1978 and BO-1919 achieved more than 99% tumor remission. We also observed that BO-1922 displayed potent therapeutic efficacy against lung adenocarcinoma A549 and human colon cancer HT-29 xenografts. These results revealed that compound BO-1922 was more potent than irinotecan against human colon cancer HT-29 cells and was as potent as irinotecan against lung adenocarcinoma A549 cells in xenograft models. Furthermore, we demonstrated that these newly synthesized derivatives possess multiple modes of action, such as the induction of DNA cross-linking, inhibition of topoisomerase I and II (topo I and topo II), and cell-cycle arrest at the S-phase.

Invited Lecturer-19

Rajesh Luthra.

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Invited Lecturer-20

Barbara Zajc, Ph.D.

Department of Chemistry, The City College and The City University of New York
160 Convent Avenue, New York, NY 10031

Education

Ph.D.	(Organic Chemistry)	E. Kardelj University of Ljubljana	1989
MS	(Organic Chemistry)	E. Kardelj University of Ljubljana	1982
BS	(Chemistry)	University of Ljubljana	1977

Appointments

2003–2012	***Associate Professor of Chemistry,*** The City College of CUNY, NY
2001–2003	***Assistant Professor of Chemistry (Substitute),*** The City College of CUNY, NY
1999	***Associate Professor of Chemistry***, University of Ljubljana, Faculty of Chemistry and Chemical Technology
1993	***Assistant Professor of Chemistr*y, University of Ljubljana, Department of Chemistry
1991	***Fogarty Fellow*,** National Institutes of Health, Bethesda, MD (until 1994, on sabbatical leave)
2000–1987	University of Ljubljana, Department of Chemistry (tenured in 1987)
1987–1977	***Research chemist***, Jo2ef Stefan Institute in Ljubljana

Awards and Merits

*	Outstanding Mentor	Recognition by The City University of New York	2012
*	Marquis Who's Who	Who's Who in Science & Engineering	2000–
*	Marquis Who's Who	Who's Who in the World	1998–
*	Fogarty Fellowship	National Institute of Diabetes, Digestive and Kidney Diseases, National Institutes of Health	1991–1994
*	Student Award	by KRKA Pharmaceuticals	1975

Professional Service

* Editorial Board member, E-Journal of Chemistry (2012)
* NSF Chemistry Panelist for *Division of Chemistry* (2011)
* Proposal reviewer for the *National Science Foundation* (2007, 2008)
* Proposal reviewer for *The American Chemical Society Petroleum Research Fund* (2004, 2005)
* Proposal reviewer for *The Research Corporation*
* Chemistry Panelist for the *PSC-CUNY 37*, *38*, *39*, *40,* and *41* grant cycles (2006–2010)
* Chemistry Panelist for *CUNY Collaborative Proposals* (2010)
* Reviewer for *PSC-CUNY* grant applications (2001–2005)
* Reviewer for the CUNY Community College Collaborative Incentive Research Grant Program (2005)
* Served as abstract reviewer for The Annual Biomedical Research Conference for Minority Students (ABRCMS) (2003, 2004)
* Reviewer for the following international journals:

The Journal of the American Chemical Society, *The Journal of Organic Chemistry, Organic Letters, Tetrahedron, Tetrahedron Letters, European Journal of Organic Chemistry, Journal of Fluorine Chemistry, Acta Chimica Slovenica*

* Undergraduate Advisor, The City College of New York (2005–2008, 2012)
* Masters Advisor, The City College of New York (2008–present)
* Member of Masters Committee (2009–present)
* Member of Organic Faculty Search Committee (2007, 2008)

Professional Affiliations

* Member of the American Chemical Society
* Member of IOTA Sigma Pi (National Honor Society of Women in Chemistry)

Doubly Functionalizable Reagents in Protio and Fluoro Julia-Kocienski Olefination

Barbara Zajc

Associate Professor,Department of Chemistry, The City College and The City University of New York
160 Convent Avenue, New York, NY 10031

Julia-Kocienski olefination is a powerful method for the synthesis of a variety of alkenes. Our research has involved development of metalation-electrophilic fluorination as a general method for synthesis of a diverse range of fluoro Julia-Kocienski olefination reagents (i.e., a fluoroolefination toolbox). One recent focus of our research has been development of bifunctionalizable Julia-Kocienski reagents that allow orthogonal functionalization. In this context, we have developed and utilized azide-alkyne cycloaddition en route to second-generation olefination reagents. A modular approach, leading to diverse vinyl and fluorovinyl triazole-based molecules, as well as approaches to fluoroenynes and fluorodienes, will be presented.

Invited Lecturer-21

4-Aminoquinoline derivatives as antimalarial agents

S. B. Katti

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A large number of drugs and biologically relevant molecules contain heterocyclic systems. The presences of hetero atoms or groupings impart preferential specificities in their biological responses. Amongst the heterocyclic systems, 4-aminoquinoline is a biologically important scaffold known to be associated with several biological activities. Some of the prominent biological responses attributed to this skeleton are antimalarial, antileisshmanial and anticancer. This diversity in the biological response profiles of 4-aminoquinoline has attracted the attention of many researchers to explore this skeleton to its multiple potential against several activities.

Historically 4-aminoquinoline based entities, particularly chloroquine (CQ), have remained the first choice in the malaria chemotherapy. The mechanistic investigations demonstrate that this class of compounds enter the food vacuole and inhibit the parasite growth by forming complex with haematin thereby inhibiting the haemozoin formation. However, development of resistance has severely limited the choice of available antimalarial drugs, which clearly highlights the urgent need of novel chemotherapeutic agents for the treatment of malaria. Contemporary biochemical studies suggest that the mechanism of resistance does not involve any change to the target of this class of drug but involves a compound specific resistance. Based on this observation a number of groups have developed short chain analogues of 4-aminoquiinoline, which are significantly active against CQ resistant strain of *P. falciparum* in vitro. On the basis of this we have designed new compounds by selectively modifying the pendant amino group of 4-aminoquinolline with a view to facilitate, (i.) their accumulation in the food vacuole, and (ii.) achieve better interaction with hematin leading to improved antimalarial activity. These results will be discussed.

Invited Lecturer-22

Regio-, chemo- and enantioselective reactions in H_2O towards synthesis of biologically Active compounds

Vishnu K. Tandon

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The impact of water in regioselective synthesis has earlier been demonstrated by us. The effect of micelles in regioselective synthesis and role of catalyst in enantioselective synthesis in H_2O shall be discussed.

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Invited Lecturer-23

Targeting the dormant 'Hypnozoites' for malaria elimination

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Division of Parasitology, CSIR-Central Drug Research Institute, Lucknow, 226001 India

Plasmodium falciparum and *P.vivax* are most common among the five species of *Plasmodium* known to cause malaria in humans. Although infection by *P.vivax* has been called the 'benign tertian malaria', geographically it is the most widely distributed cause of malaria with about 2.5 billion people at risk and perhaps one to three hundred million infections annually. Despite being a major threat to human health, *P vivax* has long been neglected and considered inconsequential in the shadow of enormous problems caused by *P.falciparum* in the African continent. *P. vivax* is especially problematic in that the infection tends to relapse, in the absence of transmission through mosquitoes. Current therapies act against the erythrocytic stages of all malarias, unless compromised due to resistance. However *P. vivax* presents an additional problem of relapse due to the activation of hypnozoites lying dormant in the liver hepatocytes. With the recent call for the development of a malaria eradication agenda, the elimination of long lasting reservoirs of infection represented by hypnozoites has become an important target. The only clinical therapy against relapses of vivax malaria is the 8-amionoquinoline drug primaquine, which however suffers the combined drawback of longer duration of treatment and risk of hemolysis in genetically sensitive cases. New approaches to the discovery of drugs targeting relapses are urgently needed as part of the eradication strategy. Discovery and development of a novel hypnozoitocidal agents is clearly the largest scientific challenge facing the malaria elimination agenda. Efforts must be made to crack the code for 'hypnozoite activation', which at present is a virtual black box. The long relative neglect of vivax malaria relapses is now being acknowledged and studies are underway to address such gaps.

Invited Lecturer-24

Role of Biotransformation in Pharmacological Actions of Drugs and in Drug Development: Significance of Cytochrome P-450 Enzymes.

Suniti Dharwadkar

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Drug metabolism is the biochemical modification –biotransformation-of pharmaceutical substances . Mixed Function Oxidise System (MFOS) is involved in biotransformation of exogenous substances (xenobiotics) including environmental pollutants and drugs. Cytochrome P450 (CYP) a terminal oxidase is the key enzyme of MFOS and plays a vital role in pharmacological actions of drugs .CYP enzyme family has received attention for drug development because of its diversified functions of metabolising wide variety of pharmaceutical agents. Various factors such as interfaces of CYP with xenobiotics and with naturally occurring compounds, drug-drug interactions and polymorphism modulate the rate of MFOs, which ultimately

determine the pharmacological action of the drug. The relationship between dietary fat type and xenobiotics metabolism is important in deciding the biological fate of the drugs. The interactions of imidazole drugs with MFOS components such as CYP and epoxide hydrolase are well studied. The understanding of the interactions of endogenous drug substrates of CYP and antifungal imidazole drugs is imperative in drug development for skin diseases. An application of pharmacogenetics to clinical practice will change the way drugs are selected. Recently the bioconversions using CYP enzymes in drug synthesis for selective oxidation and applications of bacterial and genetically engineered CYP variants have emerged as a powerful alternative. An insight in to the mechanism of drug-drug and drug-herb interactions, the newer understanding of pharmacogenic polymorphism and the novel applications of CYP will contribute to the development of safer and more efficient therapies.

Invited Lecturer-25

Prof. Laurent El Kaim

Laboratory adress : Unité Chimie et Procédés, Ecole Nationale Supérieure des Techniques Avancées, 828, boulevard des Maréchaux 91762 PALAISEAU Cedex, France
Head of the organic chemistry research group at ENSTA.
-PhD 1992 (at Ecole Polytechnique, with Pr Samir Zard)
-Associate professor at ENSTA 1993; -Professor ENSTA 2001

Main scientific interests: isocyanide chemistry, multicomponent reactions, heterocyclic chemistry… (over 100 publications)

Recent publications :

- Ugi-Smiles Couplings: New Entries to N-Aryl Carboxamide Derivatives. El Kaïm, L.; Grimaud, L. *Mol. Div*. **2010**, 14 , 855-867.
- Palladium catalyzed ring opening of furans as a route to ? ,? -unsaturated aldehydes. El Kaim, L.; Grimaud, L.; Wagschal, S. *Chem. Communication*, **2011**,47, 1887-1889.
- Palladium catalyzed ring-opening of aminocyclopropyl Ugi adducts. Dos Santos, A.; El Kaïm,L.; Grimaud, L.; Ramozzi, R. *Synlett*, **2012**, 23, 438.
- Ugi-Smiles couplings of 4-substituted pyridine derivatives: a fast access to chloroquine analogues. El Kaïm, L.; Grimaud,L.; Pravin. P. *Org. Lett*., **2012**, 7961.
- Straightforward four-component access to spiroindolines. El Kaïm, L. ;Grimaud, L. ; Le Goff, X-F. ; Menes-Arzate, M. ; Luis D. Miranda *Chem. Communication* **2011**, 8145-8147.
- New xanthate-based radical cyclization onto alkynes**.** L. El Kaïm, L. Grimaud, L. D. Miranda, E. Vieu, M.-A. Cano-Herrera, K. Perez-Labrada, *J. Chem. Soc.*, *Chem. Commun*. 2010, in press.

New cyclizations of Ugi and Ugi-Smiles adducts.

Pr Laurent El Kaim

Laboratoire Chimie et procédés, Ecole Nationale Supérieure de Techniques Avancées
32 Bd Victor, 75739 Paris Cedex 15, France
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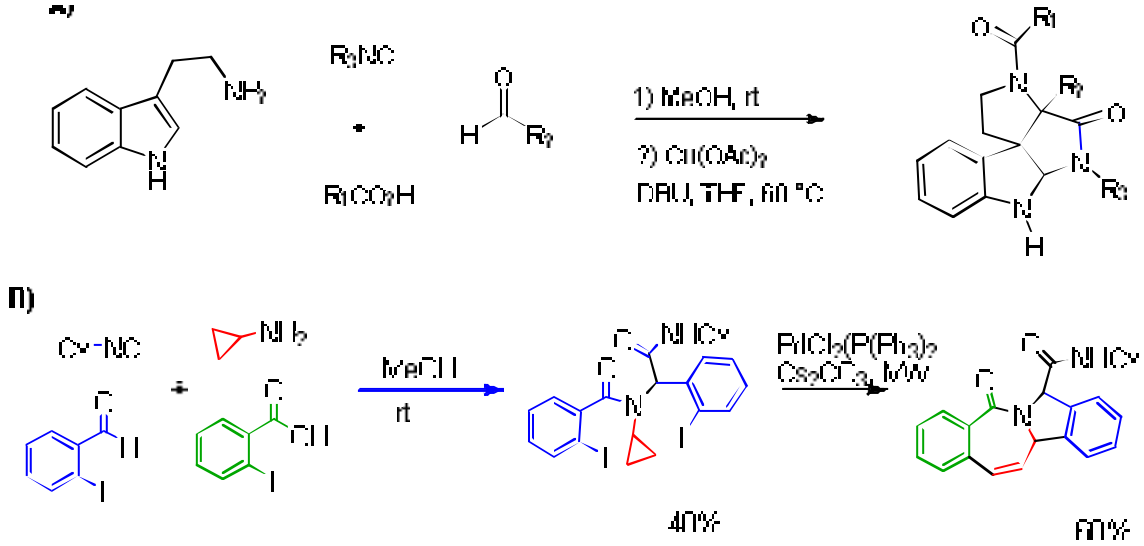
The Ugi reaction is one of the most widely recognized multicomponent reaction. Our research group has been involved in the last decade in extending the scope of Ugi reactions working mainly following two directions:

- Developping new radical and organometallic cyclizations on Ugi adducts.
- Substituting carboxylic acids in Ugi reactions by other hydroxy derivatives such as phenols, and six-membered hydroxy -heterocycles (Ugi-Smiles couplings[1]).

In the present talk, we will focus on studies on Ugi and Ugi-Smiles adducts recently performed in our group such as a copper triggered cyclization towards polycyclic indoles derivatives (**A**)[2] or a palladium triggered cascade involving cyclopropane ring-opening (**B**).[3]



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2- El Kaïm, L. ;Grimaud, L. ; Le Goff, X-F. ; Menes-Arzate, M. ; Luis D. Miranda *Chem. Communication* **2011**, 8145-8147.

3- Dos Santos, A. ; El Kaïm,L.; Grimaud, L.; Ramozzi, R. *Synlett*, **2012**, 23, 438.

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Invited Lecturer-26

Ligand-Mediated Drug Delivery Systems for Cancer Targeted Imaging and Therapy

Han-Chung Wu

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Lack of tumor specificity remains a major problem for chemotherapies in which side effects prevent the delivery of the drug dosages needed to eliminate the majority of cancer cells. Furthermore, interstitial fluid pressure (IFP) in solid tumors is higher than in normal tissues, which leads to decreased transcapillary transport of chemotherapy or anticancer antibodies into tumor tissues. Recently, we developed phage display methods to identify several novel peptides and human single chain variable fragment (scFv) antibodies that bind specifically to the plasma membrane of cancer cells. In an effort to develop targeting drug delivery systems, we used peptide-linked liposomes that carried doxorubicin to treat severe combined immunodeficiency (SCID) mice bearing human tumor xenografts. The peptide-functionalised liposomes were found to have an enhanced anti-tumor effect and reduced toxicity. Furthermore, several novel peptides were identified as being able to recognize tumor vasculature but not normal blood vessels. Antiangiogenic targeting liposomes mediated by these peptides were found to have excellent therapeutic effects. Interestingly, the targeting liposome increased therapeutic efficacy to each of these six human cancers including human lung, colon, breast, liver, pancreatic and oral cancer xenografts. The tumor site fluorescent intensity in the mice treated with targeting peptide-linked quantum dots showed higher tumor uptake and increased tumor-normal tissue ratios. In addition, *in vivo* imaging by scFv-conjugated quantum dots clearly demonstrated the potential clinical use of the scFv in tumor targeting and imaging. Our study indicates that peptide- or scFv-mediated drug delivery systems show great promise for their applications in tumor-targeted drug delivery and imaging.

Invited Lecturer-27

P7170, an Orally Efficacious, Anti-cancer Clinical Candidate Targeting PI3K/mTOR & ALK-1 Kinases

Rajiv Sharma

Department of Medicinal Chemistry
Piramal Life Sciences Ltd. Mumbai-400 063, India

Inappropriate PI3K/mTOR signalling is one of the most frequent occurrences in human cancer and is critical for tumor progression. The activation of PI3K/Akt pathway by various mechanisms is one of the most frequently observed defects in human malignancies. PI3K is therefore considered an important target for cancer treatment, and has been widely studied. Our small molecule based medicinal chemistry PI3K program has resulted in a lead candidate P7170, with excellent *in vivo* activity in multiple xenograft models. P7170 is currently in phase-I clinical trial for the treatment of cancers. In this talk, profile of P7170 a PI3K/Akt/mTOR inhibitor with unique ALK-1 inhibition, will be discussed in detail.

Invited Lecturer-28

Liabilities in drug discovery: Medicinal chemistry perspective

Sanjay Kumar

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Medicinal chemistry is a core of small molecules drug discovery and has an important role in dealing with the well-know productivity challenges in drug discovery and development. The drug discovery process is getting prolonged and expensive. It takes almost more than a decade and more than a billion dollars to discover any new drugs and its' primarily because significant liabilities identified at late stage of development leads to drug failure and thus a huge burden on the exchequer. To address these issues liability modulation has become imperative at the early discovery stage where medicinal chemistry plays a pivotal role. This talk will focus on modulation of such processes and parameters like physiochemical properties, acceptable ADME, CYPs, hERG, AMES, etc modulations towards discovery of an efficacious, druggable, potent, safe and orally efficacious molecules. Discovery of an anti-cancer orally efficacious molecule will be discussed as a case study.

Invited Lecturer-29

Design and synthesis of novel porphyrin conjugates as photochemically triggered cytotoxic agents

Dalip Kumar, Bhupendra Mishra, K P Chandra Shekar,

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Porphyrin-based macrocycles are extremely useful photosensitizers in photodynamic therapy (PDT) which is an important and promising approach for the selective destruction of localized tumors, age–related macular degeneration and various skin diseases [1]. Some of the porphyrins preferentially accumulate in malignant tissue, which upon irradiation with light of appropriate wavelength elicits highly reactive singlet oxygen-mediated cytotoxic action. In PDT, photosensitizers have low cytotoxicity until activated with visible light to generate reactive species or activates other indigenous species to be reactive and toxic [2]. Although PDT is nowadays widely used, the administration of large doses of photosensitizers to achieve the desired therapeutic effect results in generalized photosensitivity for the patient. For the enhanced delivery of photosensitizers in PDT, union of a photoactive or intercalative agent with porphyrin has emerged as one of the promising approaches [2]. In recent years, conjugation of porphyrin with carbohydrates, monoclonal antibodies, oligo-nucleotides and peptides have been explored to enhance their tumor localization [3-6]. Coupling of porphyrin with synthetic compounds or natural products with established biological significance enhances their efficacy, selectivity, and stability when compared with porphyrins alone [7]. Recently we have synthesized water-soluble cationic porphyrin conjugates and evaluated their photocytotoxicity. Details about design, synthesis and photocytotoxicity studies of porphyrin conjugates will be presented in the conference.

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Invited Lecturer-30

Asymmetric Strecker Reaction Catalyzed by Chiral Catalysts

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ABSTRACT

Development of imine functionality has been one of the most challenging area in asymmetric catalysis due to its important applications in drug discovery.[1] In this context, asymmetric Strecker reaction is one of the most direct and viable method for the synthesis of a-aminonitriles[2] (precursor to a-amino acids) by the addition of TMSCNa cyanide source to imines in the presence of chiral metal complexes[3]and organo-catalyst.[4] While acknowledging the pioneering advances in this catalytic transformation, there are still exist major challenges like maintaining the reaction conditions with low temperature, high catalyst loading, issue over recyclability and use of cyanide source. Therefore, we have developed a series of efficient recyclable chiral metal complexes and organocatalysts for highly enantioselective Strecker reaction of aromatic and aliphatic aldimines using different source of cyanidewith added advantage of catalyst reuse. The catalytic system provides an efficient protocol for the synthesis of pharmaceutically active compounds.

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Invited Lecturer-31

Plasmodium falciparum Transketolase and Purine Nucleoside Phosphorylase: Potential Drug Targets

Jitendra Kumar Saxena

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Malaria is one of the leading causes of morbidity and mortality in the Tropics. Due to emergence of drug resistance in the parasite against commonly used drugs, an urgent need exists to identify new drug targets and develop new pharmacophores with unique structures and modes of action. Targeting the parasite's metabolic pathways that lead to the formation of functional and structural components of the parasite can be a good strategy for new anti-malarial development. The pentose phosphate pathway (PPP) is an important metabolic pathway for yielding reducing power in the form of NADPH and

production of pentose sugar needed for nucleic acid synthesis. Transketolase, the key enzyme of nonoxidative arm of PPP, plays a vital role in the survival/replication of the malarial parasite. *Plasmodium* parasites are auxotrophs for purine bases and use hypoxanthine for purine salvage pathway. Purine nucleoside phosphorylase has dual cellular functions in purine salvage and polyamine metabolism. The *Plasmodium falciparum* obtains hypoxanthine either from erythrocytes or itself synthesizes by sequential action of adenosine deaminase (PfADA) and purine nucleoside phosphorylase (PfPNP). This hypoxanthine in parasite is first converted to inosine monophosphate (IMP) by the enzyme hypoxanthine-guanine-xanthine phosphoribosyl-transferase (PfHGXPRT) which is subsequently used as a precursor for synthesis of purines. 5'-methylthioadenosine (MTA), a product of polyamine metabolism has been reported to be strong inhibitor of spermine synthase, sperimidine synthase and ornithine decarboxylase. Due to its involvement in two key metabolic processes, PfPNP in *Plasmodium* is considered as an important drug target in malaria. PfTK and PfPNP were cloned, expressed and purified from bacterial cell system. The recombinant PfTk catalyzed the oxidation of donor substrates, fructose-6-phosphate (F6P) and hydroxypyruvate (HP) and p-Hydroxyphenylpyruvate showed potent inhibition of PfTk, when hydroxypyruvate was used as a substrate. The native PfTk a hexamer with subunit molecular weight of 70 kDa, upon treatment with low concentrations of guanidine hydrochloride (GdmCl) dissociated into functionally active dimers. This protein was localized in the cytosol and nucleus of the parasite. An integrated pharmacophore based virtual screening using CDRI small molecule database against PfTk lead to identification of novel and chemically diverse inhibitors. The kinetic properties of PfPNP also showed significant difference as compared to host. PfPNP accepts inosine and guanosine as substrate but not adenosine. The single tryptophan residue residing in conserved region of transition loop is present in purine nucleoside phosphorylases throughout *Plasmodium* genus. Chemical modification studies suggested that single tryptophan is essential for its activity but not for substrate binding. The observed differences in the kinetic properties of parasitic enzymes as compared to the host enzyme may facilitate designing of novel inhibitors of PfTk and PfPNP with potential anti-malarial activity.

Invited Lecturer-32

Preclinical pharmacokinetics and tissue distribution study of anti-tubercular azolyl phenyl cyclopropyl methane, S010-399, in rats

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Tuberculosis (TB) is more prevalent in the world today than at any other time in human history. India alone accounts for an estimated one fifth (21%) of all TB cases worldwide [1,2]. The compound S010-399, an azolyl phenyl cyclopropyl methane derivative, has shown anti-tubercular activity (MIC, 3.25 µM). Therefore, the pharmacokinetics and tissue uptake of of the compound was carried out in rats to develop it as a potential candidate drug.

Young and healthy male *Sprague Dawley* rats were administered a suspension formulation of the compound at 10 mg/kg oral dose. Blood, lung (target organ), liver (major metabolic site) and spleen (organ of regeneration) were collected up to 24 h post dose. A rapid, sensitive and simple HPLC assay method in rat serum, lung, liver and spleen was developed and validated as per US-FDA guidelines [3] with detection limit of 10 ng/ml and was applied for bioanalyses of S010-399.

S010-399 was found stable in SGF, SIF and rat serum. After per-oral dosing, its absorption was rapid with a peak concentration (179.9 ± 6.6 ng/ml) at 2 h and low clearance (0.003 L/h/kg; [4]). It was widely distributed to liver, lung and spleen with high mean residence time (MRT) in all four biological matrices from 8-9.6 h. S010-399 showed higher drug distribution in liver (16.62 fold), lung (4.10 fold) and spleen (2.26 fold) than serum demonstrating that it exhibits fast absorption, high volume of distribution without extra hepatic elimination and with favourable targeted tissue distribution properties. The details will be presented.

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Invited Lecturer-33

TWIN DRUGS; A DRUG DESIGN STRATEGY"

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Drugs containing two pharmacophoric groups covalently bounded in a single molecule are called TWIN DRUGS. The combination of two identical pharmacophoric entities will lead to IDENTICAL TWIN DRUGS whereas the association of two different entities will generate a NON IDENTICAL TWIN DRUGS. In twin drugs groups may combined by a linker, or a no linker or in overlap mode and are synthesized by the duplication of a group or moiety . Identical twin drugs have better efficacy than its monomeric form. The non identical twin drugs are also named as dual acting drugs or hybrid drugs because these drugs are the ligands of two different receptors or enzymes or one receptor and one enzyme .By interacting with them they produce two different actions on the same systems or two different systems. The design of such drugs called the symbiotic approach. By using this approach so many dual acting drugs have been synthesized such as Prizidilol, labetalol, D2343 etc. Such drugs have less adverse effects and better pharmacological activity spectrum. The designing of dual acting drugs is promising but is more difficult than the conventional design of drugs with single activity. A lot of success have been achieved in cardiovascular drugs but research may extended to other class of drugs such as pro-drugs, ligand bearing metal complex, molecular chameleons and gastrointestinal drugs.

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Invited Lecturer-34

Management of Impurities- a Regulatory View

Mohan Prasad

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The Control of impurities in Drug Substances and Drug Products is essential throughout development and commercialization to ensure the quality of the pharmaceutical products and safety to patients. It is a continuing concern of drug regulatory agencies and pharmaceutical industry. The international Conference on Harmonization (ICH) has issued three guidelines "Impurities in New Drug Substances", "Impurities in New Drug Products" and "Residual solvents" which provide technical requirements related to impurities for the registration of pharmaceutical Products in the European Union, United States and Japan. Similar guidelines are also published by FDA – "Guidance for Industry – ANDAS Impurities in Drug Substances", which provides recommendations on what chemistry, manufacturing, and controls (CMC) information to include regarding the reporting, identification, and qualification of impurities in drug substances produced by chemical synthesis when submitting ANDAs, DMFs and their revisions / supplements. Beside these, recently, Eur. Med. Agency- Committee for Medicinal Product for Human Use (*EMEA-CHMP)* has provided Guidelines on the limits of Genotoxic impurities. It is also becoming an integral part of fillings.

Invited Lecturer-35

Microwave Mediated Green Synthesis of Gold Nanoparticles from *Adiantum philippense* and its Cytotoxicity Study

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The present study describes the utilization of the aqueous extract of the aerial parts of *"Adiantum philippense"* for the synthesis of gold nanoparticles (GNPs). *A. philippense* is a fern well known for its medicinal value worldwide (Malviya et al. 2012, Sikarwar et al. 2008). The synthesis reactions of gold nanoparticles were carried out under the microwave irradiation conditions. Instrumental analysis of the reaction products revealed physico-chemical characteristics typical of gold nanoparticles. UV-Vis spectral analysis confirmed the presence of Surface Plasmon Resonance (SPR) absorption spectra with sharp and distinct SPR peaks. Transmission Electron Microscopy (TEM), X-ray diffraction (XRD) and Fourier Transform Infra Red (FTIR) were carried out respectively for the morphological, cryastallinity and functional group analysis of the synthesized gold nanoparticles respectively. Mouse fibroblast cell line L929 was used for the cytotoxicity studies of gold nanoparticles. MTT (3-[4, 5-dimethylthiazole-2-yl]-2, 5-diphenyl tetrazolium bromide) and acridine orange/ethidium bromide (AO/EtBr) live/dead cell assays were done for quantitative and qualitative estimation of cytotoxicity of the synthesized gold nanoparticles (Mossaman 1983).

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Invited Lecturer-36

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Invited Lecturer-37

Prof. Anamik Shah

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Professor Dr. Anamik Shah is working as a senior most faculty member at Department of Chemistry, Saurashtra University. After appointment as a faculty member in 1983, for last 29 years, Professor Anamik Shah is teaching Organic Chemistry, Medicinal Chemistry, Environmental Chemistry, and Pharma Analytical Chemistry. He is currently President of Indian Society of Chemists and Biologists, Lucknow, where he has also served as Vice President during 2002 to 2010.

Professor Shah is one of the Professors in the National University System to work on several industry-academic research projects. Research group of Prof. Shah has successfully worked on **16 National and International Research Projects**. Professor Shah is currently running research programs of more than 8 Crore of Department of Science & Technology, Government of India, National Institute of Health (NIH)-USA, Department of Biotechnology, Department of Atomic Energy, National Medicinal Plant Board - New Delhi, on diversified fields of medicinal chemistry research on anti HIV, anticancer and antitubercular drug discovery, preservation of molecular diversity, etc.

Professor Shah has pursued his degree of Doctor of Philosophy (Chemistry) in year 1983, Master of Science in year 1977, and Special LLB in year 1988. He is awarded by International Scientific Partnership Foundation, Russia, along with many others.

Professor Shah has guided 55 doctoral students and team of 18 research scholars is currently working under his guidance. He has more than **118 research publications** in national and international journals of well repute; **one book** and **one book chapter**, as well as **five patents** on his name.

In last 35 years, Professor Shah has served on various key-positions in more than 20 research and social organizations; Expert and Selection Committee Member in UGC Plan Committees and Major Research Projects (Chemistry), Selection committee of Lectures, Readers, Professors of various Universities in Gujarat and other states, Scientists of CSIR affiliated Research Institutes, Various Prestigious Science Awards of Gujarat (Vikram Sarabhai Award) and other state awards of India. He has referee-ship of more than 20 national and international universities. Professor Shah has been bestowed with honorarium guide-ship in Banasthali University, Rajasthan, and Kadi University, Gandhinagar.

SYNTHESIS AND PHARMACOLOGY OF PYRANOQUINOLINE ANALOGUES AS ANTI-CANCER PROMISING LEADS

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Several natural products related Synthetic analogues are up-coming as potential drug candidates in recent Drug Discovery regime. In last few years, our research focus was aimed at Natural Product 'Like' scaffolds. Several series of such compounds were identified in collaboration with pharmaceutical companies as a potential candidate.

Pyranoquinoline has emerged as one of the most promising scaffold in our study. Current talk is exploration of synthesis of various Pyranoquinolines & their systematic pharmacological outcome. The entire work establishes newer leads in cancer treatment. In addition to this, some recent results will also be discussed relevant to the talk.

Invited Lecturer-38

Spermicides: Local contraceptive agents

Anil Kumar Dwivedi

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According to an estimate, ~40% of all pregnancies that occurred worldwide were unintended, which strongly indicates that the available methods of contraception are insufficient to cater the unmet need of millions of couples. Nonoxynol-9 (N-9), a detergent with potent spermicidal properties is used as an active ingredient in many spermicidal preparations. However, multiple use of N-9 spermicide may cause irritation to the vagina and rectum, increasing the chance of HIV and STD infections in users. The other surfactants like octoxynol-9, menfegol (TS-88) and benzalkonium chloride that have been used as spermicides, also non-specifically disrupt cell membranes and are, therefore, cytotoxic to a wide range of cell types including Lactobacilli, which facilitate the maintenance of an optimal environment in the vagina. *Trichomonas vaginalis*, the most prevalent non-viral sexually transmitted infection (STI) that is transmitted along with fertile sperm is gaining resistance against the US-FDA approved drug metronidazole. Anti-trichomonal spermicides can tender dual protection by inactivating fertile sperm as well as *Trichomonas*. Consequently, a non-detergent spermicidal microbicide is perhaps the most viable way of providing contraception with prophylaxis against STDs.

Our Institute has developed and licensed a vaginal contraceptive cream (CONSAP) which contains saponins isolated from the fruit pericarp of the plant *Sapindus mukorossi* as the active ingredient. Though safer than N-9, saponins exhibit a similar non-specific surfactant action on sperm. Consequently efforts were made to target sperm with more specific, mechanism-based molecules directed against specific target(s) on sperm cells, and which resulted in several series of potent non-detergent spermicidal structures. These series will be discussed in details.

Invited Lecturer-39

Professor N C Desai,

Dean, Faculty of Science & Head, Department of Chemistry, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar

(a) Name: Nisheethkumar Chhotalal Desai

(b) Designation: Dean, Faculty of Science, Professor & Head, Department of Chemistry, Department of Chemistry, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar

(c) Areas of Specialization: (i) Organic and Medicinal Chemistry,
(ii) Green Chemistry
(ii) Intellectual Property Rights & Management,
(iv) Entrepreneurship in Academic Institutes

(d) Research Experience & Training: 33 Years research experience

Publications: 67 Research Papers in National & International Journals of repute: (i) International-37 (Thirteen papers)-List attached (ii) National 30

Ph. D. Guidance: Thirty one (31) students have successfully pursued and obtained Ph. D. degree – List attached separately, and currently six students (06) are pursuing research for their Ph. D. Degree,

(e) Distinguished Award:

(i) Received prestigious **Career Award for Young Scientist** from University Grant Commission, New Delhi, for a period of 3 years (1995-1998) which carried Rs. 2 lakhs for further research on HIV and Cancer chemotherapy.

(ii) Sanctioned a special grant of Rs. 7 lakhs by University Grants Commission, New Delhiunder its scheme for one time grant to Professors of Science Departments of various universities under "UGC-BVSR". UGC offers grant to faculty members in recognition of providing guidance to a minimum of 15 full time Ph.D. students

(f) Liaison with other Research Institutes:

(i) National Institute of Health, Maryland, (U.S.A.) (ii) American Cynamide (U.S.A.), (iii) BASF Aktienquesellscharg (Germany), (iv) B V Patel Pharmaceutical Education Research Centre, (PERD Centre) Ahmedabad, (v) Central Drug Research Institute, Lucknow, (vi) Alembic Reaearch Centre, Vadodara,

(g) Reorganization by Chancellor:

(i) Nominated as the Chairman of the Search Committee for the selection of the panel for the Vice Chancellor, Saurashtra Other important initiative: Served as the Coordinator-FIST program, funded by DST, Govt of India

Invited Lecturer-39

SMALL & HYBRID HETEROCYCLIC SCAFFOLDS AS SMART ANTIMICROBIAL AGENTS

N C Desai

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Combat against bacterial infections has resulted in the development of a wide variety of antibiotics. After years of misuse and overuse of antibiotics, bacteria are becoming antibiotic resistant, resulting in a potential global health crisis. Antibacterial and antifungal diseases are very common all over the world. Currently used antimicrobial agents are not effective due to the resistance developed by the microbes. And therefore, it is an ongoing effort to synthesize new antimicrobial agents. In order to overcome this rapid development of drug resistance, new agents should preferably consist of chemical characteristics that clearly differ from those of existing agents. In drug developing programs, an essential component of the search for new leads is the synthesis of molecules, which are novel yet resemble known biologically active molecules by virtue of presence of critical structural features. To cater this need, the development of "small molecules", term that indicates biological active small molecules, has had a big impact on drug discovery process. Hybrid molecules, which are defined as chemical entities with two or more structural domains having different biological functions and dual activity have emerged as a beneficial tool against infectious disease specifically against those which are resistant or possess MDR, indicating that a hybrid molecule might act as two distinct pharmacophores. In order to obtain new antimicrobial agents that are affordable and able to avoid the emergence of resistant strains, we have developed small and hybrid molecules with a probable dual mode of action (a "double-edged sword") able to kill multiresistant strains. In continuation to this, we are involved in the synthesis of such small and smart hybrid heterocyclic scaffolds like imidazole, quinoline, 4-thiazolidinone, oxadiazole, azetidinone, quinazolinone, pyrazole, triazole derivatives and clubbing them with other potentially active pharmacophores and have received very interesting results on bacteria and fungi. These small and hybrid molecules will play a vital role for the generation of lead molecules.

Invited Lecturer-39A

Prof A. K. Goswami

Department of Chemistry, Mohan Lal Sukhadia University, Udaipur

Dr. A. K. Goswami, is Professor and Head, Department of Chemistry, M. L. S. University Udaipur and Director Industrial Chemistry Department. He has worked on co-ordination chemistry since last 30 years and has more than 85 papers and 10 reviews to his credit. The research field he is working are analytical reagents, hydroxytriazenes, bio-inorganic chemistry, computer aided drug designing, etc. Recently, he is working on photo-chemical and mechano-chemical synthesis of triazene compounds of bio-importance. He has 25 Ph.D. students to his credit and 10 students are working for their Ph. D. under his guidence.

Hydroxytriazines – Potential Drug Intermediates

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Hydroxytriazines have been exhaustively studied in our laboratory for the last many years starting from their analytical applications as metallochromic and complexometric reagents for transition metals, they have been found useful as bio-active molecules. They have been screened for antibacterial and antifungal as well as anti-inflammatory activities and have been found to possess mo derate to excellent activities. The most interesting fact about the compounds is that triazene group is a very suitable moiety for photo-chemical and mechano-chemical synthesis of important compounds such as dyes, and drugs. The present talk is about the future strategy of synthesis of drugs through green route, i.e. mechano-chemical synthesis and mechano-photochemical synthesis.

Invited Lecturer-39B

Prof B. L. Ahuja

Department of Physics, Mohan Lal Sukhadia University, Udaipur

Since 1984, Prof. B.L. Ahuja is actively engaged in the field of Compton scattering, environmental physics, X-ray fluorescence, magnetism, engineering of materials for a variety of applications like solar cells, spintronics compounds and band structure calculations. He was awarded BOYSCAST fellowship (1992-93) by DST, New Delhi to work at University of Warwick, U.K. for development of instrumentation for synchrotron radiations. Prof. Ahuja has designed, fabricated and commissioned the first Indian 20 Ci ^{137}Cs Compton spectrometer and the first-ever lowest intensity 100 mCi ^{241}Am Compton spectrometer in M.L. Sukhadia University, Udaipur, Rajasthan. For the measurement of high resolution and magnetic Compton profiles, he has worked at Universite de Paris-sud (LURE), France; Daresbury Synchrotron Source, U.K.; KEK, Japan; European Synchrotron Radiation Facility (ESRF), Grenoble, France and Super Photon Ring 8 GeV (SPring-8), Japan. Prof. Ahuja has supervised 21 students for their Ph.D. degree and presently 9 students are working with him for the same. Prof. Ahuja has executed several R&D projects funded by DST, CSIR, UGC, AICTE, UGC-DAE-CSR, BRNS and DRDO, etc. He is coordinator of DST-FIST (level-2, grant Rs.three crores) programme. He has got working collaborations with 31 institutes within India and abroad. He has published about 118 papers in very reputed international journals and about 130 publications in conference-proceedings, etc. In addition, Prof. Ahuja is also a reviewer of several topmost international journals (like PRB, PRL) and is associated with many scientific societies in different capacities. Presently, Prof. Ahuja is Head of Physics Department in M.L. Sukhadia University, Udaipur (Rajasthan). He is also Vice-president of Indian Society of Radiation Physics.

Use of Compton scattering in characterization of technologically important compounds

B.L. Ahuja

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ABSTRACT

Compton scattering (CS) is a well proven technique to obtain the electron momentum density in variety of materials [1, 2]. In CS, one measures the double differential scattering cross-section which is used to extract the Compton profiles. Compton profile which is projection of electron momentum density along the scattering vector is related to electron wave functions deduced from different quantum mechanical models. Therefore, this technique is helpful in direct verification of electronic structure and chemical bonding, etc. in variety of compounds.

In this talk, starting from the basics of charge and magnetic CS, I will present the charge Compton profile of 1,3,5-Trinitro-1,3,5-triazinane ($C_3H_6N_6O_6$, also known as RDX), octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine ($C_4H_8N_8O_8$, also known as HMX) and ammonium nitrate (NH_4NO_3). The Compton data will be compared with the linear combination of atomic orbitals. The data will be analyzed in terms of hydrogen bonding, bond length and bond angle, etc. The potential of magnetic Compton profiles will be illustrated on the basis of spin momentum densities, electronic and magnetic properties of some ferrites and manganites.

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Invited Lecturer-40

Bio-catalytic Synthesis of Amphiphilic Polymeric and Dendritic Architectures for Biomedical Applications

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In response to the increasing need for easy-to-prepare and versatile nanotransport systems for biomedical applications, the importance of polymers and dendrimers has been well recognized. Polymers are most widely used as pharmaceutical carriers in drug delivery, and a considerable amount of research has been directed toward the use of natural and synthetic polymers as polymeric drugs and drug delivery systems. On the other hand dendrimers represent a key stage in the ongoing evolution of macromolecular chemistry and research in this field has experienced an exponential development in both academic and technological areas.

We have developed a chemo-enzymatic methodology for the synthesis of functionalized amphiphilic polymers and dendritic architectures based on glycerol, polyglycerol, polyethylene glycol (PEG), and alkyl / aryl moieties that aggregate in aqueous medium to form nanospheres. We used poly(ethylene glycol)s, (PEGs) because they are known to be biocompatible, nontoxic, and water-soluble. Glycerol and polyglycerol on the other hand are the most versatile and valuable chemical substances and are utilized in a variety of commercial products with no known adverse pharmacological or environmental effects. Moreover, they exhibit good chemical stability and inertness under biological conditions. The molecular encapsulation of small hydrophobic drugs using these polymeric / dendritic materials has been studied.

Invited Lecturer-41

Metabonomics : A Platform for Testing Toxicity

Neeraj Sinha

Senior Principal Scientist, Division of Toxicology, Central Drug Research Institute, Lucknow

During past two decades several techniques viz. **'Genomics'**, '**Proteomics'** and **'Metabonomics'** - collectively constitute an **'Omic World',** are being developed to understand and investigate the complex metabolic consequences of disease processes, toxic reactions and diagnosis. Although, Genomics and Proteomics measurements respond to the administration of Toxic agents and tried to explain the fundamental nature of many toxicological reactions and disease processes, thus triggering interest in the field of 'Omics' yet, it is difficult to relate findings to classical toxicological end points and hence influence the drug attrition rate. Under such condition the third technology i.e. 'Metabonomics' offers a complementary approach that gives information on whole organism functional integrity over time after drug / chemical exposure.

Among several spectroscopic methods **bioanalytically**, NMR is the powerful means of generating multivariate metabolic data. NMR has the advantages of being non-destructive, applicable to intact biomaterials, and intrinsically more information rich with respect to the determination of molecular structures, especially in complex-mixture analyses. Target tissues or processes, and biomarkers, can be identified by characteristic changes in the pattern of concentrations of endogenous metabolites in biofluids and tissues too that relate to the site and mechanism of toxicity. During conference, two experiments viz. **Nephrotoxicity** and **Hepatotoxicity** conducted at our laboratory will be presented and discussed.

Invited Lecturer-42

Ram S. Mohan

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Education: B.Sc. Honors in Chemistry (**1985**), Hansraj College, Delhi, India; M.S., Organic Chemistry (**1987**), University of Delhi, India; Ph.D., Chemistry (**1992**), University of Maryland, Baltimore County (Advisor: Dr. Dale Whalen); Post-doctoral Research Associate (Advisor: Dr. Robert M. Coates), (**1992-1994**), University of Illinois at Urbana-Champaign, Urbana, IL.

Academic Positions: Visiting Assistant Professor of Chemistry (Coker College, SC) **1994-1996**, Started at Illinois Wesleyan University in **1996** as Visiting Assistant Professor; Currently The Earl H. and Marian A. Beling Professor of Natural Sciences and Professor of Chemistry.

Awards and Honors:

- ***Fulbright-Nehru Visiting Lecturer to India*** (October 2012 to March 2013)
- ***Chemist of The Year 2011 (***Illinois Heartland Section of The American Chemical Society)
- **International Union of Pure and Applied Chemistry (IUPAC) Young Observer Award:** (Selected to represent the USA to participate as a young observer in the IUPAC General Assembly and Congress),Glasgow, United Kingdom(**August 2009**).

- **Pfizer Inc. (St. Louis Green Chemistry Team) Green Chemistry Award** ($5000) in recognition of contribution to green chemistry education and research (**2008**).
- **Top-50 most cited articles" as published in *Tetrahedron* 2007-2008**": Reactivity of ionic liquids. Chowdhury, S.; Scott, J. L.;Mohan, R. S.*Tetrahedron* **2007,** *63,* 2363-2389.
- **Top-50 most cited articles" as published in *Tetrahedron* 2004-2007**": Bismuth compounds in organic synthesis. Bismuth nitrate catalyzed chemoselective synthesis of acylals from aromatic aldehydes." Aggen, D. A.; Arnold, J. N.; Hayes, P. D.; Smoter, N. M.; Mohan, R. S. **2004,** *60*, 3675.
- **Nominated by the U.S. National Research Council and Selected by CERC (Chairmen of the European Research Council's Chemistry Committee)** to attend a workshop on use of Lanthanides in organic synthesis, Belgium(February **2006**).
- **International Union of Pure and Applied Chemistry (IUPAC) Young Observer Award:** (Selected as one of eight from the USA to participate as a young observer in the IUPAC General Assembly and Congress),Ottawa, Canada(August **2003**).
- **The University of Maryland, Baltimore County 2002 Distinguished Alumni Award.**
- **Henry Dreyfus Teacher-Scholar Award for 2001** (Awarded by The Camille and Henry Dreyfus Foundation, Inc.) (Award amount: $60,000) (November **2001**).

Research Activities, Funding and Impact on Undergraduates: Dr. Ram Mohan has received a total of approximately $1,200,000from various funding agencies that include The National Science Foundation, American Chemical Society-Petroleum Research Fund, Research Corporation and Illinois Wesleyan University. Dr. Ram Mohan is an editorial board memberof *The Open Catalysis Journal* (Bentham Publishers) and *Green & Sustainable Journal*.He has published sixty refereed papers, supervised the research of over 100 undergraduatesand atotal of 75 undergraduates have been co-authors on refereed manuscripts. His research focuses on development of environmentally friendly organic synthetic methodology using bismuth and iron compounds. In addition he is interested in ionic liquids, and in development of discovery-oriented laboratory experiments for organic chemistry.

Environmentally friendly organic synthesis using bismuth (III) and iron (III) compounds

Ram S. Mohan

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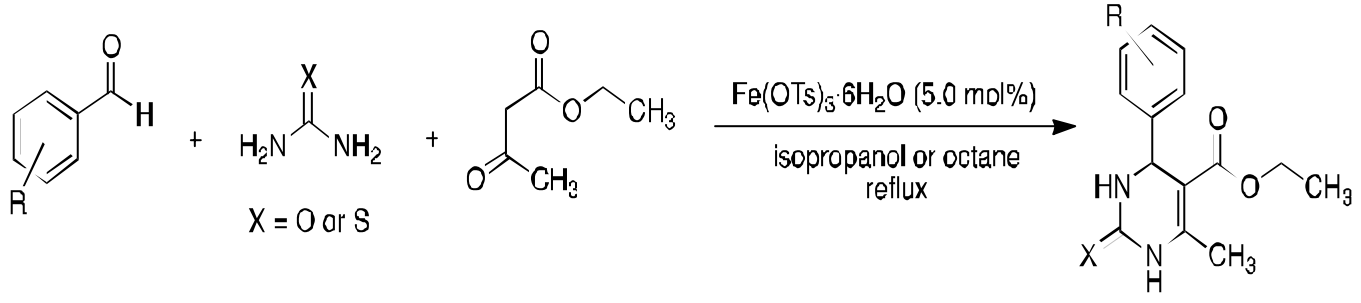
With increasing environmental concerns, the need for nontoxic and noncorrosive catalysts has assumed increased importance. In this context bismuth(III) compounds are especially attractive because they are remarkably non-toxic, non corrosive and inexpensive. Bismuth compounds are also reasonably tolerant of small amounts of moisture and are stable in air. The utility of bismuth(III) compounds as Lewis acid catalysts in organic synthesis will be illustrated. In addition we have recently demonstrated the utility of iron(III) tosylate in organic synthesis. The Biginelli reaction is typically catalyzed by a Brønsted or Lewis acid. But many of these catalysts such as $BF_3{\cdot}Et_2O$ and $AlCl_3$ are corrosive and/or toxic. We now report that iron(III) tosylate is a versatile catalyst for the Biginelli reaction (Scheme 1). These results will also be presented.

Scheme 1



Invited Lecturer-43

Design and Development of thioxothiazoles as A2A receptor antagonists in the therapy of Parkinson's Disease

Pratibha Mehta Luthra

Dr. B.R. Ambedkar Centre for Biomedical Research, University of Delhi, Delhi 110007, India

Parkinson's Disease is a neurodegenerative motor dysfuntion caused due to loss of dopaminergic neurons in nigrostriatal pathways resulting in the reduction of striatal dopamine concentration. The primary symptoms of Parkinson's disease result from greatly reduced activity of dopamine-secreting cells caused by cell death in the region of the substantia nigra (Obeso et al., 2008). The blockade of A_{2A}Rs in striatopallidal neurons diminish postsynaptic effects of dopamine depletion and reduce the motor deficits of PD (Aoyama et al., 2000; Chen et al. 2003). A_{2A}R antagonists inhibit basal ganglia pathway from striatum to thalamus via globus pallidus pars externa, subthalamic nucleus (STN), and internal pallidum (Gerfen 1992). Numerous structurally different A_{2A}R antagonists such as xanthine compounds based on the structures of naturally occurring methylxanthines, caffeine and theophylline (Fredholm et al. 1997) and non-xanthine compounds SCH58261 and ZM241385, have been reported. However, xanthine compounds such as KW6002 were mostly unsuccessful in clinical trials and nonxanthines such as SCH58261 suffered from lower selectivity, poor solubility and poor pharmacokinetic profile. Previously, thiazolotriazolopyrmidines and thiazolopyrimidines have been developed as novel and selective A2AR antagonist (Mishra et al. 2010 and Luthra et al. 2010). The structure based approach has been used to develop thioxothiazoles as novel and selective A2AR antagonists.

1. Aoyama, S., Kase, H., Borrelli, E., 2000. Rescue of locomotor impairmentin dopamine D2 receptor-deficient mice by an adenosine A2A receptor antagonist. J. Neurosci. 20, 5848–5852.
2. Obeso JA, Rodríguez-Oroz MC, Benitez-Temino B (2008). "Functional organization of the basal ganglia:therapeutic implications for Parkinson's disease". *Mov. Disord.* 23: 548–59
3. Chen J-F, Fredduzzi S, Bastia E, Yu L-Q, Moratalla R, Ongini E, Schwarzschild MA (2003) Adenosine A2A receptors in neuroadaptation to repeated dopaminergic stimulation: implications for the treatment of dyskinesia in Parkinson's disease. Neurology 61(suppl.6) s74-s81
4. Fredholm BB, Arslan G, Johansson B, Kull B, Svenningsson P (1997) Adenosine A_{2A} receptors and the actions of caffeine. In: The Role of Adenosine in the Nervous System, pp. 51-74. Ed. Y. Okada. Elsevier Science, Amsterdam.
5. Luthra, PM, Mishra CB, Jha PK, Barodia SK (2010). Synthesis of novel 7-imino-2-thioxo-3,7dihydro-2H-thiazolo [4,5-d] pyrimidine derivatives as adenosine A2A receptor antagonists Bioorganic & Medicinal Chemistry Letters 3 :1214-1218.
6. Mishra CB, Barodia SK, Prakash A, Kumar JBS, Luthra, PM (2010). Novel 8-(furan-2-yl)-3-substituted thiazolo [5,4-e][1,2,4]triazolo[1,5-c] pyrimidine-2(3H)-thione derivatives as potential adenosine A_{2A} receptor antagonists. Bioorg Med Chem 18: 2491-500.

Invited Lecturer-44

Conventional vs. Non-conventional Energy Sources for Organic Transformations in Aqueous Media

M. S. Shingare

Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431 004. (M. S.) India.
Email: msshingare@yahoo.com

The green chemistry revolution is providing an enormous number of challenges to those who practice chemistry in industry, education and research. With these challenges however, there are an equal number of opportunities to discover and apply new chemistry, to improve the economics of chemical manufacturing and to enhance the much-tarnished image of chemistry.

The challenge for chemists and others is to develop new products, processes and services following ideal synthesis that achieve combination of a number of environmental, health and safety, and economic targets. This requires a new approach which sets out to reduce the materials and energy intensity of chemical processes and products, minimize or eliminate the dispersion of harmful chemicals in the environment and maximize the use of renewable. One of the thrust areas for achieving this target is to explore alternative reaction conditions and reaction media to accomplish the desired organic/chemical transformations with minimized by-products or waste as well as eliminating the use of conventional organic solvents, wherever possible.

In this context, some appealing aspects that lead to achieve more sustainable routes in organic synthesis *either by* conventional or non-conventional routes are desired. In such a scenario, water has been emerged out as a solvent of choice, because of its unique characteristics. Consequently, some non-conventional strategies have also appeared as the alternate heating and activation methods to carry out organic synthesis, which include microwave and ultrasonic irradiations. These techniques overcome some of the problems associated with excessive or wasteful heating.

Invited Lecturer-44A

Prof G. L. Talesara

Department of Chemistry, Mohan Lal Sukhadia University, Udaipur

Personal Details

Academic Qualifications

M.Sc. (1972) : M.B College, University of Udaipur

Gold Medalist (1st Position in University)

B.Sc. (1970) : SMB Govt College, Nathdara, Rajasthan University **1st Position in College**

Ph.D. (1984) : University of Udaipur, Udaipur (Raj.)

Subject: "Studies on amino-oxy and related compounds".

Work Experience & Positions Held

- Selected by RPSC at 1st Position (1973) as **Lecturer** in chemistry
- Worked as Lecturer in Govt Colleges under **Directorate of College Education, Raj.(Sep.1972-Feb.1986) 13 years and 6 months**
- Joined ML Sukhadia University in 1986 as **Assistant Professor**.
- Selected for **Associate Professor (1990)**
- Selected for **Professor(May 2007)**
- Joined as Head, University, Department of Chemistry MLS University, Udaipur (from Dec17, 2007)
- Teaching Experience UG 37 years & PG 23 Years.

Research Profile

Ph. D. Awardees : 29

Research Publications : 111

Publications in the Journals Including

- Medicinal Chemistry Research (Springer-link).
- J of Sulfur Chemistry (Taylor & Francis,)
- J of P, S, Si & Related Elements (Taylor & Francis),
- Enzyme Inhibition and Medicinal Chemistry (Taylor and Francis)
- ARKIVOC (USA)
- AFINIDAD (SPAIN)
- E Journal of Chemistry
- J of Pharmaceutical Science

- Indian J of Chemistry (NISCAIR, CSIR)
- J of Indian chemical Society
- J of Indian council of Chemists
- Indian Journal of Heterocyclic Chemistry
- Research J of Chemistry & Environment

Conferences, Seminars & Symposia

Participated and Presented Papers:

- Convention of chemists Indian Chemical society Bhopal 2012
- International conference at **Malaysia** (kualalumpur) june 2012
- International conference of ICC, **Bangkok** (Thialand), June 2011.
- Indian Council of Chemists, Panjab University, **Chandigarh** Dec2010
- UGC Symposium ,Banasthali University, **Banasthali** Oct 2010
- Indian Council of Chemists, North Gujarat University, **Patan (Gujarat)**. 2009
- ICS, M. G. Institute of Applied Sciences, **Jaipur (Rajasthan).** Dec, 2007
- Indian Council of Chemists, Mumbai University, **Mumbai,** Dec, 2006
- Joint International Conference of American Chemical Society-CSIR- AOCCB IICT, **Hyderabad (AP).** Jan, 2006,
- International Congress of Chemistry and Environment (ICCE-05), **Indore ,** 2005
- Energy Environment and Chemical Industries, MLSU, **Udaipur,** Dec., 2005
- Petrotech Society "Academia Industry Interface", **INSA– New Delhi**, Sept., 2005
- Newer Dimensions in Chemistry, MLSU, **Udaipur (Raj.).** Dec., 2004
- Indian Council of Chemists Mumbai University, **Mumbai** Oct., 2004,
- Indian Council of Chemists IIT- **Roorkee (Uttranchal)** , Oct., 2003,
- Indian Chemical Society (38th Convention), **Jodhpur (Raj.)** Dec., 2001,
- World Chemistry Congress **Brisbane, Australia,** July2001
  - ❖ International Union of Pure and Applied Chemists 38th Congress
  - ❖ Asian Federation of Medicinal Chemistry Congress 2001
  - ❖ Federation of Asian Chemical Societies 9th Congress
- International Conference of Chemistry (ICS), **Calcutta (West Bengal) ,**1999
- Indian Council of Chemists **Mangalore, (Karnataka).** Dec., 1997
- Indian Council of Chemists, **Aurangabad (Maharastra).** Oct., 1997
- Indian Council of Chemists, **Srinagar (J&K).** Nov., 1982
- Indian Council of Chemists, **Agra (UP).** Sept., 1981.

Invited Lectures Delivered

- International conference at **Malaysia (kualalumpur)** june 2012
- International conference of ICC, **Bangkok** (Thialand), June 2011.
- Indian Council of Chemists, Panjab University, **Chandigarh** Dec2010.
- UGC Symposium ,Banasthali University, **Banasthali** Oct 2010
- Indian Council of Chemists, North Gujarat University, 2009, **Patan (Gujarat).**
- ICS, M. G. Institute of Applied Sciences, Dec, 2007, **Jaipur.**
- Indian Council of Chemists, Dec., 2006, **Mumbai.**
- Newer Dimensions in Chemistry", Dec., 2004, MLSU, **Udaipur.**
- Recent trends in Chemical Science", MLSU, Dec., 2000, **Udaipur.**
- ISCB (Drug Research Scenario of 21st Century), Jan., 2000, CDRI, **Lucknow.**

Chaired at National and International level : 19 Times

Judge (expert) for young scientist award: 10 Times

Referee for Journals including:

- Synthetic Communication (Tailor & Francis)
- Tetrahedron Letters
- Natural Product Research
- Elsevier Journals
- Medicinal Chemistry Research (Springer-link)
- Main group of chemistry (Taylor & Francis)
- Arkivoc (USA)
- Indian Journal of Chemistry (NISCAIR)
- Journal of Indian Chemical Society
- Indian Journal of Heterocyclic Chemistry
- African Journal of Pharmaceutical Sciences

Member of Editorial Board Of Journal:

- Journal of Chemistry and Environment
- International Journal of Chemical Sciences

Vice-president:

- Indian Council of Chemists : 2004-07
- Indian Council of Chemists : 2007-09

Member of Academic council and Advisory Board:

- Mewar University, Chittorgarh

Associate Editor:

- Journal of Indian Chemical Society

Member of Executive Committee:

- Indian Council of Chemists: 2002-04

Council Member:

- Indian Chemical Society: 2007-09

Fellow Member:

- International Union of Pure and Applied Chemistry (**IUPAC-AFM**)
- American Chemical Society (**ACS-Member -AFM**)
- International Congress of Chemistry and Environment (F**ICCE**)
- Indian Science Congress Association (F**ISCA)**
- Indian Chemical Society (F**ICS)**
- Indian Society of Chemists and Biologists (F**ISCB)**
- Indian Council of Chemists (F**ICC)**

Abstract for invited lecture

Target to develop chemotherapeutically potential heterocyclic class of privileged scaffolds and their combinations, prediction of their bioactivity, biological evaluation and their structure activity relationships

Prof. (Dr.) G L Talesara

Former Professor and Head, Deptt. of Chemistry, M L Sukhadia University, Udaipur (Raj.) 313001
Email:- glntalesara@yahoo.com

Current interest of medicinal scientist is focused on design and synthesis of new drugs with improved pharmacokinetic properties. Heterocycles have been recognized as privileged structure and emerged guiding principal for modern drugs discovery. Intense global efforts have been under way to develop biologically active material from various heterocycles. Heterocyclic chemistry has increased great prominence over the years in the field of research. The presences of one or more hetero atoms within the carbocyclic analogues are accountable for better biological activities in the heterocycles. It has been apprised that more than 60-65% of all published research paper and reviews of chemical studies deal in one or another way with heterocyclic systems.

Each year witness the growing inclusion of many thousands of heterocyclic compounds in literature, both on account of their intrinsic chemical interest and on the basis of their therapeutic, biological and industrial potential. Heterocyclic chemistry is vast and important subject. About half of the ten million or so compounds recorded in the chemical abstracts are heterocyclic. Heterocyclic chemistry persist an interesting psychology as it is a vast and expanding area of chemistry due to multiple applications of their compounds. It may fairly be said that heterocyclic pharmacy chemistry although cover one third of all organic chemistry, has started to receive as much attention as it merits. During the past 20 years, a multitude of novel bio-active heterocycles have being developed and several of these are being considered as therapeutic agents for various disease. Our most important contribution have been towards the synthesis of library of new bioactive heterocycles, their combination and to investigate their efficacy as antimicrobial, anti inflammatory, anti cancer, anti tumor, anti tubercular, anti malarial, cardiovascular, angiogenic, anti HIV, anti viral etc.

In this context we synthesized one rings, two rings, three rings and more than three rings, free, fused and attached heterocycles viz: azetidinones, pyrazoles, thiazoles, oxazoles, imidazoles, triazoles, pyridines, pyrimidines, piperazines, pyrazines, quinolines, quinazolens, qindoles, morpholines, diazepines, phenothiazines, carbazoles, phathalazines, nepthyridines, (as singal name heterocycles), thiazoloquinazolines, pyrazoloimidazoles, thiazolopyridines, thiazoloxazoles, thiazolothiazolidinone, pyrazolopyrazoles, thiazolopyrimidines, thiazolopyrazines, thiazolodiazepines, isoniazidothiazolidinones, isoniazidopyrimidines, pyranopyrazoles, pyrazolopyrimidines, pyrazolopyridines, pyrazolodiazepines, quinolothiazolidinones, isoxazolodiazepines, pyrazoloisoxazoles, thiazoloisoxazoles, (as two rings), pyrido-pyrimidinyl-imidazolidinones, imidazolo-pyrazolo-thiazolidinones, thiazolo-pyrimidinyl-thiazolidinones, pyrimido-thiazolo-thiadiazoles, pyrazolo-pyrido-pyrimido-quinazolines (as three and more rings). Synthesized compounds have been estimated for prediction of various pharmacological activities and also evaluated for possible and available bioactivities.

Invited Lecturer-44B

P. P. Yadav

Medicinal and Process Chemistry Division, CDRI, Lucknow

Brief Biography:

Prem Prakash Yadav did his B. Sc. and M.Sc from Allahabad University. He received Ph.D in 2005 from Dr. R. M. L. Avadh University, Faizabad on the research work carried out at Medicinal and Process Chemistry Division of Central Drug Research Institute. While completing his Ph.D in 2005 he joined Medicinal and Process Chemistry Division of Central Drug Research Institute as Junior Scientist followed by promotion to his present position of Scientist. He was awarded by DAAD postdoctoral fellowship (2008-2009) in the research group of Prof. Hartmut Laatsch of University of Goettingen, Germany, where he worked on identification of biologically active secondary metabolites from marine Actinomycetes. He has to his credit 25 publications, 1book chapter and two patents with an average impact factor of 3.4 and h-index of 9. Presently his research group is involved in medicinal chemistry research on malaria and diabetes.

CURRICULUM VITAE

Name: **Dr. Prem Prakash Yadav**

Designation: Scientist

Institute: Medicinal and Process Chemistry Division

CSIR-Central Drug Research Institute,

Chattar Manzil Palace, Lucknow-226 001, INDIA.

Date of Birth: March 06, 1978

Sex Male

Married Yes

Telephone: 0522-2612411-18, Ext. 2496(Office)

Fax: 0522-2623405/2623938

E-mail: pp_yadav@cdri.res.in

Academic Qualifications

B. Sc.	1999	University of Allahabad, India
M. Sc. (Chemistry)	2001	University of Allahabad, India
Ph. D. (Chemistry)	2005	Dr R. M. L. Avadh University, Faizabad, India Supervisor: Dr. Rakesh Maurya, Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Chattar Manzil Palace, Lucknow-226 001 India

Title of Thesis: Phytochemical investigation of medicinal plants and chemical transformation of bio-active natural products.

Professional activities:

08/2001 - 03/2005	Research Scholar, CSIR-Central Drug Research Institute, Lucknow, India
04/1999 –05/2005	Senior Research Fellow,CSIR-Central Drug Research Institute, Lucknow, India
13/05/05 – 12/05/08	Jr. Scientist, Medicinal & Process Chemistry Division, Central Drug Research Institute, Lucknow, India.
09/06/08 – 01/10/09	Deputed to Goettingen University, Germany, for Post Doctoral Project on Microbial Metabolites funded by DAAD.
13/05/08 – CONT.	Scientist, Medicinal & Process Chemistry Division, Central Drug Research Institute, Lucknow, India.

Academic Honors/Awards:

2008-09 Awarded DAAD Post Doctoral fellowship

2005 Awarded Senior Research Fellowship (CSIR, New Delhi).

2001 Qualified GATE-2001.

List of Publications

1. Ranjani Maurya, Awakash Soni, Devireddy Anand, Makthala Ravi, Kanumuri S. R. Raju, Isha Taneja, Niraj K. Naikade, S. K. Puri, Wahajuddin, Sanjeev Kanojiya, **PP Yadav**, "Synthesis and Antimalarial activity of 3,3-spiroanellated 5,6-disubstituted-1,2,4-trioxanes". ***ACS Med. Chem. Lett.*** Article ASAP **DOI:** 10.1021/ml300188t. (IF 2011: 3.35)

2. Makthala Ravi, Devireddy Anand, Ranjani Maurya, Parul Chauhan, Niraj K. Naikade, Sanjeev K. Shukla, **Prem P. Yadav**, "Synthesis of 1,2,4-Trioxepanes and 1,2,4-Trioxanes via H_2O_2-Mediated Reaction of Tertiary Carbinols". ***Synlett* 2013**, 24, 173. (IF 2011: 2.71)

3. Bandana Chakravarti, Ranjani Maurya, Jawed Akhtar Siddiqui, Hemant Kumar Bid, S. M. Rajendranc, **Prem P. Yadav**, Rituraj Konwar. "*In vitro* anti-breast cancer activity of ethanolic extract of *Wrightia tomentosa*: Role of proapoptotic effects of oleanolic acid and urosolic acid". ***Journal of Ethnopharmacology*** 2012, 142,72-79. (IF 2011: 3.014)

4. Ranjani Maurya , Anuj Srivastava , Priyanka Shah, Mohammad Imran Siddiqi, S. M. Rajendran, Anju Puri, **Prem P. Yadav**. "ß-Amyrin acetate and ß-Amyrin palmitate as antidyslipidemic agents from Wrightia tomentosa leaves". ***Phytomedicine*** 2012, 19, 682-685. (IF 2011: 3.268)

5. Ranjani Maurya, Makhtala Ravi, Snehlata Singh, **Prem P. Yadav**. "A review on cassane and norcassane diterpenes and their pharmacological studies". ***Fitoterapia*** 2012, 83, 272. (IF 2011: 1.848)

6. Jaiswal, N., **Yadav, P. P**., Maurya, R., Srivastava, A.K., Tamrakar, A.K. "Karanjin from Pongamia pinnata induces GLUT4 translocation in skeletal muscle cells in a phosphatidylinositol-3-kinase-independent manner" ***European Journal of Pharmacology*** 2011, 670, 22–28. (IF 2011: 2.516)

7. Muna Ali Abdalla, **Prem P. Yadav**, Birger Dittrich, Anja Schueffler, Hartmut Laatsch."ent-Homoabyssomicins A and B, Two New Spirotetronate Metabolites from *Streptomyces* sp. Ank 210". ***Organic Letters*** 2011, 13(9), 2156-2159. (IF 2011: 5.862)

8. Tamrakar, A.K, Jaiswal, N., **Yadav, P. P**., Maurya, R., Srivastava, A.K. "Pongamol from Pongamia pinnata stimulates glucose uptake by increasing surface GLUT4 level in skeletal muscle cells" ***Molecular and Cellular Endocrinology*** 2011, 339 (1-2), 98-104. (IF 2011: 4.192)

9. Adaramoye, O.A., Sarkar, J., Singh, N., Meena, S., Changkija, B., **Yadav, P. P**., Kanojiya, S., Sinha, S. "Antiproliferative Action of Xylopia aethiopica Fruit Extract on Human Cervical Cancer Cells" ***Phytotherapy Research***, 2011, 25(10), 1558-1563. (IF 2011: 2.086)

10. Akanksha, **Prem P. Yadav**, Arvind K. Srivastava, Rakesh Maurya. "Synthesis of analogues of antihyperglycemic lead karanjin" ***Medicinal Chemistry Research*** 2011, 20, 1465-1472. (IF 2011: 1.271)

11. **Prem P. Yadav**, Vimal Nair, Birger Dittrich, Anja Schueffler, Hartmut Laatsch. "Lucknowlides A and B, tricyclic ketal-lactone metabolites from terrestrial *Streptomyces Sp*." ***Organic Letters*** 2010, 12(17), 3800-3803. (IF 2011: 5.862)

12. **Prem P. Yadav**, Ranjani Maurya, Jayanta Sarkar, Ashish Arora, Sanjeev Kanojiya, Sudhir Sinha, M.N. Srivastava, Ram Raghubir. "Cassane Diterpenes from Caesalpinia bonduc" ***Phytochemistry*** 2009, 70, 256–261. (IF 2011: 3.351)

13. "*Terminalia arjuna* a sacred medicinal plant: phytochemical and pharmacological profile" Sunyana Jain, **Prem P. Yadav**, Vikrant Gill, Neeru Vasudeva, Neelam Singla. **Phytochemistry Reviews** 2009, 8, 491-502. (IF 2011: 4.333)

14. Sanjeev Kanojiya and **Prem P. Yadav**. "Fragmentation patterns of newly isolated cassane butenolide diterpenes and differentiation of stereoisomer by tandem mass spectrometry" ***Journal of Mass Spectrometry***; 2008, 43, 1413-1420. (IF 2011: 3.268)

15. Akhilesh K Tamrakar, **Prem P. Yadav**, Priti Tiwari, Rakesh Maurya, Arvind K. Srivastave. Identification of pongamol and karanjin as lead compounds with antihyperglycemic activity from *Pongamia pinnata* fruits. ***Journal of Ethnopharmacology***, 2008, 118, 435-439. (IF 2011: 3.014)

16. G. Bhatia, A. Puri, R. Maurya, **Prem P. Yadav**, M. M. Khan, A. K. Khanna, Jitender Kumar Saxena. Anti-dyslipidemic and antioxidant activities of different fractions of Pongamia pinnata (lin.) fruits. ***Medicinal Chemistry Research*** 2008, 17:281–289. (IF 2011: 1.271)

17. **Prem P. Yadav**, Ashish Arora, Hemant K. Bid, Ritu R. Konver, Sanjeev Kanojia. New cassane butenolide hemiketal diterpenes from the marine creeper Caesalpinia bonduc and their antiproliferative activity ***Tetrahedron Lett.*** 2007, 48, 7194–7198. (IF 2011: 2.683)

18. G. Ahmad, P. K. Mishra, P. Gupta, **Prem P. Yadav**, P. Tiwari, A. K. Tamrakar, A. K. Srivastava and R. Maurya. Synthesis of novel benzofuran isoxazolines as protein tyrosine phosphatase 1B inhibitors. ***Bioorganic & Medicinal Chemistry Letters***, 2006, 16, 2139-2143. (IF 2011: 2.554)

19. R. Maurya, **Prem P. Yadav**. Furanoflavonoids: An Overview. ***Natural Product Reports*** 2005, **22**, 400 - 424. (IF 2010: 9.79)

20. **Prem P. Yadav**, Prasoon Gupta, A. K. Chaturvedi, P. K. Shukla, Rakesh Maurya. "Synthesis of 4-hydroxy-1-methylindole and benzo[b]thiophen-4-ol based unnatural flavonoids as new class of antimicrobial agents" ***Bioorganic and Medicinal Chemistry,*** 2005, **13**, 1497-1505. (IF 2011: 2.921)

21. **Prem P. Yadav**, Ghufran Ahmad and Rakesh Maurya**.** An efficient route for commercially viable syntheses of furan- and thiophene-anellated ß- hydroxychalcones. ***Tetrahedron Letters***, 2005**, 46**, 5621-5624. (IF 2011: 2.683)

22. R. Maurya, L. R. Manhas, P. Gupta, P. K. Mishra, G. Singh, **Prem P. Yadav**. "Amritosides A, B, C and D: clerodane furano diterpene glucosides from *Tinospora cordifolia*" ***Phytochemistry***, 2004, **65**, 2051-2055. (IF 2011: 3.351)

23. R. Maurya, R. Singh, M. Deepak, S.S. Handa, **Prem P. Yadav**, P. K. Mishra. "Constituents of *Pterocarpus marsupium*: an ayurvedic crude drug" ***Phytochemistry*** 2004, 65, 915–920. (IF 2011: 3.351)

24. G. Ahmad, **Prem P. Yadav**, R. Maurya. "Furanoflavonoid glycosides from *Pongamia pinnata* fruits" ***Phytochemistry*** 2004, 65, 921–924. (IF 2011: 3.351)

25. **Prem P. Yadav**, G. Ahmad, R. Maurya. "Furanoflavonoids from *Pongamia pinnata* fruits" ***Phytochemistry*** 2004, 65, 439–443. (IF 2011: 3.351)

Chapter in a Book: 1

1. Rakesh Maurya, Geetu Singh and **Prem P. Yadav**. "Antiosteoporotic Agents from Natural Sources". ***Studies in Natural Product Chemistry***, 2008, 35 (C), 517-548.

Patent: 2

1. "Isolation and synthesis of novel furano and pyranoflavonoids as antidiabetic agents" R. Maurya, A. Goel, T. Narender A. K.Srivastava, A. K. Rastogi, S. C. Agarwal, S. M. Rajendran, C. Nath, C. M. Gupta, **P. P. Yadav**, Shweta, M. Dixit, P. Tiwari, B. K. Tripathi. **Patent No. 199NF2005/IN**, 528DEL2006 date of filing 28.02.2006.

2. "Novel 3, 3-spiroanellated 5, 6-disubstituted -1, 2, 4-trioxanes as antimalarial agents and a process for the preparation thereof" **P. P. Yadav**, S. K. Puri, R. Maurya, A. Soni. **Patent Application No. 008NF2011/IN**, **0265DEL2011** date of filing 04.02.2011.

- **Total Impact factor of publications**: 85.251
- **Average Impact factor of publications**: 3.41
- **Total no of Citations** (***Google scholar***): 281
- ***h*-index:** 9

Spiroannelated 1,2,4-trioxanes as antimalarials

Prem P. Yadav

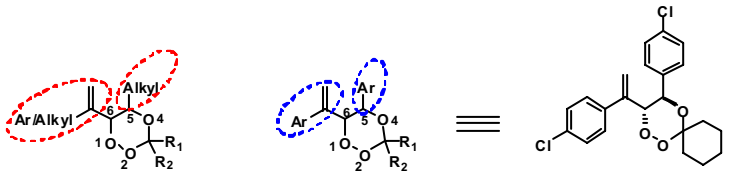
Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow-226001, India
e-mail: pp_yadav@cdri.res.in

ABSTRACT

Malaria is a major parasitic disease of the tropics, around 215 million people are affected and an estimated 6,55,000 people died of malaria in 2010.[1] The situation has worsened due to drug resistance to common chemotherapeutic agents. Synthetic trioxanes containing 1,2,4-trioxane pharmacophore of artemisinin has been a key area of research since discovery of antimalarial lead molecule artemisinin from *Artemisia annua*.[2] Artemisinin and its derivatives have been thoroughly investigated for their efficacy against malaria parasite and also their peroxide specific mode of action. Initial efforts to resolve the issues associated with artemisinin like poor bioavalibility, short plasma half-life and solubility led to discovery of more potent antimalarial derivatives such as arteether, artemether and artesunate.[3] Good safety and fast action of theses derivatives made them the drugs of choice for activity against drug resistant strains of *P. falciparum.* On the grounds of peroxide group specific antimalarial activity of artemisinin many synthetic peroxides have been synthesized and tested for their efficacy and were found to show promising antimalarial activity as compared to artemisinin. The crucial step in the synthesis of these oxygen heterocycles is the introduction of the hydroperoxy group. In the reported methods, this has been achieved by (i) H_2O_2

mediated reaction of acetophenone derived carbinols (ii) Photooxygenation of allylic or homoallylic alcohol (iii) Lewis acid-catalyzed opening of oxetanes by hydrogen peroxide and (iv) Ozonolysis of enol ethers. Synthetic peroxides class has been represented by 1,2-dioxanes(endoperoxides), 1,2,4-trioxanes, 1,2,4-trioxolanes, 1,2,4-trioxepanes and tetraoxanes. Some of these synthetic peroxides have advanced to the clinical development stage.

Looking forward towards trioxanes as potential candidates for antimalarial drug development we have explored novel substitution in spiroannelated 5,6,-disubstitured 1,2,4-trioxanes. The reported 1,2,4-trioxanes have a substitution at C-6 owing to the ease of synthesis via ene reaction of allylic alcohols with singlet oxygen. They have synthesized number of compounds based on allylic alcohols derived from wittig/reformatsky product of various phenyl methyl ketones and displayed the importance of an aryl vinyl substitution at C-6 of the 1,2,4-trioxane moiety, along with effect of different substituents in the aromatic ring. The results from Singh el al., led us to keep the C-6 phenyl vinyl part as such in our 1,2,4-trioxane and incorporate another aromatic ring at C-5 position.[4]. The best active compound identified in the exercise was found to be twice as active as the reference drug ß-arteether and can serve as a lead for further optimization.



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(2) D L Klayman, Science 228, 1985, 1049.

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Invited Lecturer-44C

Vineet Kumar

Chemistry Division, Forest Research Institute, Dehradun

RESEARCH 20 years experience as Scientist in Indian Council of Forestry Research and Education (An Autonomous Council of Ministry of Environment and Forests, Govt. of India)

Publications

55 including 1 World Patent and 1 Indian Patent

R Gross and **Vineet Kumar**. Acrylation of Hyaluronic Acid. PCT/US07/63671 dated March 09, 2007 International Publication No: WO 2007/10678 A2 dated 20 September 2007. EP 2007758243 **granted 30.12.2009** US No 12280187 (22.08.2008); AU No. 2007226690 (14.08.2008); CA 2647481 (11.09.2008); CN 200780009291.9 (16.09.2008); JP No 2009500563 (03.09.2008)

Vineet Kumar. An improved binding material for incense sticks (Agarbattis). Indian Patent Application No. 1802/ Del /2011 dated 24.06.2011

50 Scientific papers and reviews published in internationally recognized journals such as *Journal of Chemical Research, Carbohydrate Polymers*, *Planta Medica*, *Phytochemical Analysis*, International Journal of Biological Macromolecules, Food Hydrocolloids, *Journal of Applied Polymer Science*, *Journal of Macromolecular Science*, *Indian Journal of Chemistry*, *Journal of Medicinal and Aromatic Plants*, *Chemistry and Industry*, *Journal of Indian Chemical Society*, etc.

BOOKS CO-EDITED (3):

***Trends in Carbohydrate Chemistry* - Vol. IV (1999) and Vol. V (2000)**

Surya International Publications, Dehradun, India

Natural Products and Biodiversity: Chemistry and Utilization, F R I, Dehradun (2009)

Thesis supervised

Ph.D., Prerana Badoni (2012) Antimicrobial activity of *Sapindus mukorossii*

Ph.D., Puja Goyal (2009) Chemical modification of Tamarind Kernel Powder.

Ph.D., Vikas Rana (2007) Chemical investigation of *Dalbergia sissoo* Roxb. leaf polysaccharide.

Ph.D., Anjana Rani (2005) Structural investigation of *Cassia tora* Linn. seed polysaccharide.

Ph.D., Brij Raj Sharma (2004) Chemical modification of polysaccharides for industrial applications.

Ph.D., Shipra Nagar (continuing) Isolation and structural investigation of polysaccharide from *Tinospora sinensis*.

Ph.D., Meenakshi Naudiyal (continuing) Structural studies of *Hippophae salicifolia* polysaccharide.

Ph.D., Pradeep Kumar (continuing) Chemical investigation of *Vitex negundo* polysaccharide.

Ph.D., Ajeet K Lakhera (continuing) Chemical characterization of *Acacia tortilis* gum exudates and its comparison with other important Acacia gums.

Ph.D., Shanti Devi (continuing) Chemical examination of *M. coromandelianum* for biologically important polysaccharide

M. Tech. (Bangalore Univ.) B.V. Bharti (1996) Studies on dyeing of cotton, silk and wool with natural dyes.

M. Tech. (Bangalore Univ.) P.M. Reddy (1996) Natural dyes isolation and application on different fibers.

In addition, guided a number of JRF/Associates for implementation of different projects sponsored by different agencies viz. NMPB, DBT, DST, ICFRE, etc.

Technology Transfers

With an emphasis on 'transfer of technology from laboratory to common man, the technologies developed in laboratory on 'substitute of binding material for incense stick making' (patent filed) and 'reshaping of gums' were transferred to four entrepreneurs by charging license fees.

Invited Talks

>25 presentations at conferences/symposia as KEY NOTE ADDRESS, PLENARY LECTURES, LEAD LECTURES and INVITED TALKS in key national and international conferences at IICT, Hyderabad; CDRI, Lucknow; NIPER, Mohali; Delhi University, Delhi; CFTRI, Mysore; Bogor University, Bogor (Indonesia), Punjabi University, Patiala, H.N.B. Garhwal University, Srinagar, Bhavnagar University, Bhavnagar, Indian Institute of Natural Resins and Gums, Ranchi, etc.

Fellowships

Visiting Scientist at Department of Chemical and Biological Sciences, POLYTECHNIC UNIVERSITY, New York sponsored by NOVOZYMES, Denmark from 2004- 2006.

DAAD Postdoctoral fellow at Department of Pharmaceutical Chemistry, ALBERT LUDWIGS UNIVERSITY, Freiburg for the year 2000-2001 sponsored by German Academic Exchange Service, Bonn.

Academic awards and distinctions

Awarded with the prestigious 'National Award for Excellence' by Indian Council of Forestry Research and Education under the category 'Young Scientists Award' for the period ending 2008

Awarded Research Fellowship of the Council of Scientific and Industrial Research through National Examination Test (NET) held jointly by CSIR and University Grant Commission, New Delhi

1st position in University in M.Phil Chemistry and awarded GOLD MEDAL

Awarded Lion Joseph's scholarship in M.Sc. by Maharashi Dayanand University.

Awarded University Scholarship by Maharashi Dayanand University, Rohtak at undergraduate.

Recipient of prestigious NATIONAL SCHOLARSHIP awarded by Govt. of India.

Appreciations Work during my stay at Polytechnic University, New York was highly appreciated by Prof. Richard A. Gross, Director, Centre for Biocatalysis and Bioprocessing of Macromolecules, Polytechnic University, New York. Similarly Prof. A. W. Frahm, Head, Department of Pharmaceutical Chemistry, Albert Ludwigs University, Freiburg has high opinion of my contribution during my stay at Freiburg.

Projects undertaken and completed

Refining of process for detoxification of Jatropha seed oil (sponsored by ICFRE, Dehradun)

Phytochemical examination of bioactive agents from plants of therapeutic value (Sponsored by NMPB, New Delhi)

Utilization of economic potential of *Lantana camara* (sponsored by DST, New Delhi)

Studies on *Sapindus mukorossii* fruits for their utilization (sponsored by ICFRE, Dehradun)

Novel chemoenzymatic technology to prepare food fibre from Guar/*Cassia tora* gums(sponsored by DBT, New Delhi)

Chemical modification of Hyaluronic acid (sponsored by Novozymes, Denmark)

Conformational analysis of biflavanonols and flavone-chromone moiety of *Cratoxylum neriifolium* (sponsored by DAAD, Bonn)

Structural characterization of *Dalbergia sissoo* leaf polysaccharide (sponsored by ICFRE, Dehradun)

Chemical modification of galactomannan gums (sponsored by ICFRE, Dehradun)

Chemical medication of Tamarind Kernel Powder (sponsored by ICFRE, Dehradun)

Structural characterization of *Cassia tora* seed gum (sponsored by ICFRE, Dehradun)

Utilization of *Taxus baccata* for its bioactive principles (sponsored by ICFRE, Dehradun)

Isolation of santalins from Red Sanders (*Pterocarpus santalinus*) (sponsored by IWST, Bangalore)

Development of natural dyes from Forest biomass (sponsored by IWST, Bangalore)

Skills **Polysaccharides Investigation:** Extensive experience in isolation of polysaccharides, purification, isolation of oligosaccharides, methylation, G.L.C. analysis, and characterization of oligosaccharides and polysaccharide using chromatographic and advanced spectroscopic techniques (1 and 2D NMR viz ^{1}H-^{1}HCOSY, HMBC, HMQC, NOESY, ROESY, TOCSY etc).

Phytochemical Investigation: Extensive experience in isolation and characterization of natural products viz. extraction, slurry preparation, isolation and characterization of pure compounds using different chromatographic and advanced spectroscopic techniques (1 and 2D NMR viz ^{1}H-^{1}HCOSY, HMBC, HMQC, NOESY, ROESY, TOCSY etc).

Polysaccharides Modification: Introduction of different functional groups in polysaccharides using enzymatic/chemical routes. Synthesis *via* condensation, free radical polymerization. Chemo-enzymatic modification of hyaluronic acid, galactomannans (*Cassia tora*, guar gum), xyloglucans (tamarind kernel powder), pectins etc.

Organic Synthesis: Multi-step synthesis, heterocyclic molecules design and synthesis, polymer synthesis, air sensitive reactions, compounds isolation, purification, identification, isolation and handling of compounds in small quantities.

Instrumental Techniques: (^{1}H-, ^{13}C-, 2D) NMR, FT-IR (transmittance, DRIFT, ATR, Photoacoustics) and UV-Visible spectroscopy. Expertise in traditional & modern separation and analytical techniques, i.e. column (open air and flash), thin layer (analytical and preparative), gas (GC), high performance liquid (HPLC, analytical and preparative) and gel permeation chromatography (GPC).

Invited by Director General, Indian Council of Agriculture Research (ICAR), New Delhi to be a member of the Research Advisory Committee (RAC) of one of their constituent institute namely Indian Institute of Natural Resins and Gums, Ranchi to guide the research in the area of polysaccharide chemistry. Similarly

I am honorary member of the Academic Council of Fragrance and Flavour Development Centre, Kannauj

RAC and Academic Council member

Member of the Editorial Board of the Journal 'Trends in Carbohydrate Research'. In addition, referee for the evaluation of papers in leading journals viz. 'European Polymer Journal', 'Carbohydrate Polymers', 'Bioresource Technology', Fitoterapia. Natural Products Research, , 'Journal of Applied Polymer Science', 'Journal of Macromolecular Science: Pure and Applied Chemistry', etc

Editorial Board Member and Referee

Teaching P.G. Diploma in Aromatechnolgy and M.Sc. in Wood Science and Technology students at Forest Research Institute, University for last 12 years. In addition, I am the Course Coordinator and Nodal Officer of the course P.G. Diploma in Aromatechnology. I am member of Academic Council, Research Advisory Committee, Research Degree Committee of FRI University. Actively involved in all works related to paper setting, entrance examinations, conducting practical examination etc. of FRI University.

TEACHING

In addition to research work and teaching, following facilities were developed in the department based the sponsored projects and in-house funded projects:

Facilities developed

1. Lyophilizer
2. Rheometer
3. Refrigerated ultracentrifuge
4. FT-IR spectrophotometer
5. UV-visible spectrophotometer
6. Deep Freezer

List of Publications

A. Patents:

1. R Gross and **Vineet Kumar**. Acrylation of Hyaluronic Acid. PCT/US07/63671 dated March 09, 2007 International Publication No: WO 2007/10678 A2 dated 20 September 2007. EP 2007758243 **Granted 30.12.2009** US No 12280187 (22.08.2008); AU No. 2007226690 (14.08.2008); CA 2647481 (11.09.2008); CN 200780009291.9 (16.09.2008); JP No 2009500563 (03.09.2008)
2. **Vineet Kumar.** An improved binding material for incense sticks (Agarbattis). Indian Patent Application No. 1802/ Del /2011 dated 24.06.2011

B. Research papers

3. **Vineet Kumar,** V. Rana, and P.L. Soni (2013). Molecular Weight Determination and Correlation Analysis of *Dalbergia sissoo* Polysaccharide with Constituent Oligosaccharides. Phytochemical Analysis 24, 75-80.
4. M. Jindal, **Vineet Kumar**, V. Rana and A.K. Tiwary (2013). Physico-chemical, mechanical and electrical performance of bael fruit gum-chitosan IPN films. Food Hydrocolloids 30, 192-199.
5. M. Jindal, **Vineet Kumar**, V. Rana and A.K. Tiwary (2013). An insight into the properties of *Aegle marmelos* pectin–chitosan cross-linked films. International Journal of Biological Macromolecules 52, 77– 84
6. M. Jindal, **Vineet Kumar**, V. Rana and A.K. Tiwary (2013). *Aegle marmelos* fruit pectin for food and pharmaceuticals: Physico-chemical, rheological and functional performance Carbohydrate Polymers Carbohydrate Polymers (in press doi:10.1016/j.carbpol.2012.12.012).
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8. V. Rana, **Vineet Kumar**, and P.L.Soni (2012). Structural characterization of an acidic polysaccharide from *Dalbergia sissoo* Roxb. Leaf polysaccharide. Carbohydrate Polymers 90, 243-250.
9. **Vineet Kumar**, P. Goyal and P.L. Soni (2012). Preparation of Quaternary Ammonium Compound of Tamarind Kernel Powder. Trends in Carbohydrate Research 4 (2), 47-53
10. **Vineet Kumar**, Sanjay Naithani and Deepika Pandey (2011). Optimization of reaction conditions for grafting of a-cellulose isolated from *Lantana camara* with acrylamide. Carbohydrate Polymers 86, 760-768.

11. V. Rana and **Vineet Kumar** (2011). Linkage Analysis in a Trisaccharide from Dalbergia by Methylation and Periodate Oxidation Methods. International Journal of ChemTech Research 3 (1), 483-487.
12. **Vineet Kumar** (2010). Carboxymethycellulose: A Versatile Industrial Polymer. ENVIS Forestry Bulletin 10(1), 76-83.
13. Y.C. Tripathi, **Vineet Kumar** and Rashmi (2010). Herbal antioxidants for Health- A move towards nature. ENVIS Forestry Bulletin 10(1), 1-8.
14. V. Rana, **Vineet Kumar** and P.L. Soni (2009). Structure of the oligoscacharides isolated from *Dalbergia sissoo* leaf polysaccharide. Carbohydrate Polymers 78 (30), 520-525
15. Puja Goyal, **Vineet Kumar** and P. Sharma (2009). Ce (IV) initiated graft copolymerization of Acrylonitrile onto Tamarind Kernel. Journal of Applied Polymer Science 114 (1), 377-386
16. **Vineet Kumar** (2009). Bioactive polysaccharides from plants. Natural Products and Biodiversity: Chemistry and Utilization' Forest Research Institute, Dehradun 117-123
17. **Vineet Kumar** (2009). Oils and Fats, Chapter 15, contributed in Training Manual on Capacity Building of Communities Involved in Sustainable Forest Management published by Forest Research Institute, Dehradun and Department for Environment, Food and Rural Affairs (DEFRA), UK p151-159.
18. P. Goyal, **Vineet Kumar** and P. Sharma (2008). Cyanoethylation of Tamarind Kernel Powder *Starch (Starke)* **60(1),** 41-47
19. P. Goyal, **Vineet Kumar** and Pradeep Sharma (2008). Graft Copolymerization of Acrylamide onto Tamarind Kernel Powder in the presence of ceric ion Journal of Applied Polymer Science **108 (6),** 3696
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22. B.R. Sharma, **Vineet Kumar** and P.L. Soni (2004). Chemical modification of guar gum: carbamoylethylation. *Carbohydrate Polymers* **58:** 449
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26. P.L.Soni, R. Dayal, **Vineet Kumar** (2003). Environment friendly technologies for sustainable utilization of non-wood forest products. *Indian Forester* **129**: 853
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28. B.R. Sharma, **Vineet Kumar** and P.L. Soni (2003). Ce(iv)-ion initiated graft copolymerization of methyl methacrylate onto guar gum. *Journal of Macromolecular Science, Part A, Pure and Applied Chemistry* **40**: 49.
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31. **Vineet Kumar,** Anjana Rani and P.L. Soni (2000). Recent development in galactomannan applications. *Trends in Carbohydrate Chemistry* **6**: 129.
32. Amit Bhatt, **Vineet Kumar** and P.L. Soni (2000). Pyrolytic cleaved products of starch- dextrins: prospects and perspectives. *Trends in Carbohydrate Chemistry* **6**: 107.
33. B. R. Sharma, **Vineet Kumar** and P.L. Soni (1999). Preparation of flocculants using seed gums for industrial needs. *Trends in Carbohydrate Chemistry* **5**: 75.
34. J. Mohan and **Vineet Kumar** (1998). Synthesis of novel imidazo[1,2-*a*]-s-triazolo-1,3,4-thiadiazoles. *Indian J. Heterocyclic Chem.* **8**: 73.
35. **Vineet Kumar** and B.V. Bharti (1998). *Mangifera indica* bark: a source of natural dye. *American Dyestuff Reporter* **87**: 18.

36. J. Mohan and **Vineet Kumar** (1998). Synthesis, Stereochemistry and antimicrobial activity of pyrazolo[3',4':4,5]-thiazolo[3,2-*b*]-s-tetrazines. *Indian J. Heterocyclic Chem.* **7:**297.

37. J. Mohan and **Vineet Kumar** (1998). Synthesis, stereochemistry and antimicrobial activity of spiro[cydopentane-1',7(8H)-(6H)-pyrazolo[3;4':d]thiazolo[3',2':b]-s-tetrazines] *Indian J. Heterocyclic Chem.* **7:** 233.

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40. J. Mohan and **Vineet Kumar** (1998). Synthesis and bioactivity of 2,3-dinydro-4H-[1,3]thiazino[3^1,2^1:2,3]as-triazino[5,6-b]indoles and quinoxalino[2',3':4,5]thiazolo[3,2-b]indolo[2,3 e]-as-triazine and their isomeric systems. *Indian J. Chem.* **37B**: 95.

41. K.S. Thegarajan, K.H.S. Narayana, **Vineet Kumar**, A.N.R. Lochan and R. Kumar (1997). Chemical modification of Eucalyptus hybrid oil. *J. Med. Aromatic Plants* **19**: 669.

42. J. Mohan and **Vineet Kumar** (1997). Synthesis and antimicrobial activity of thiazolo [3',2':2,3]-as-triazino[5,6-*b*]indoles and isomeric thiazolo[2',3':3,4]-as-triazino[5,6-*b*]indoles. *Indian J. Chem.* **36B**: 1030.

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45. K. S. Thegarajan and **Vineet Kumar** (1995). Essential oils of commercial importance in India-utilization and future prospects. *Indian Perfumer* **39**: 49.

46. K.H.S. Narayana and **Vineet Kumar** (1995)**.** Structure and industrial application of tetraethanol methylene diamine. *Research and Industry* **40**: 293.

47. J. Mohan, V. Singh, **Vineet Kumar** and S. Kataria (1994). Reaction of 2-aminothiadiazoles with ∝-haloketones in presence of [hydroxy (p-tosyloxy) iodo] benzene. *Indian J. Chem.* **33B**: 686.

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49. J. Mohan, V. Singh and **Vineet Kumar** (1993)**.** Synthesis and antimicrobial activity of thiazolo[3,2-*b*]-s-triazoles and isomeric [2,3-*c*]-s-triazoles. *Indian J. Heterocyclic Chem.* **3**: 47.

50. J. Mohan, V. Singh and **Vineet Kumar** (1993). Heterocyclic Systems Containing Bridgehead Nitrogen Atom: Synthesis and antimicrobial activity of spiro [bicyclo(2.2.1)heptane-2,3'-(4'H)-[2'H]-thiazolo[3,2-*b*]-s-tetrazines] and spiro[bicyclo (2.2.1) heptane-2,3'(4'H)[2'H]pyrazolo [3',4':4,5]thiazolo[3,2-*b*]-s-tetrazines] and spiro[bicyclo(2,2,1)heptane-2,3'(4'H)[2'H] pyrazolo[3',4':4,5] thiazolo[3,2-*b*]-s-tetrazines. Novel and hitherto unknown heterocyclic systems. *Indian J. Chem.* **32B**: 593.

51. J. Mohan and **Vineet Kumar** (1992). Heterocyclic systems containing bridgehead nitrogen atom: synthesis and antimicrobial activity of spiro[cyclohexane-1',7-(8H)-(6H)-pyrazolo (3,4-*d*) thiazolo [3,2-*b*]-s-tetrazines]. *Indian J. Heterocyclic Chem.* **2**: 99.

52. J. Mohan, P. Verma, and **Vineet Kumar** (1992). Bridghead nitrogen heterocycles: facile synthesis and antimicrobial activity of thiazolo [3,2-*b*]-s-tetrazines and pyrazolo[3',4':4',5] thiazolo[3,2-*b*]-s-tetrazines. *J. Indian Chem. Soc.* **6**: 693.

53. **Vineet Kumar**. 'Novel Eco-friendly Processes for Sustainable Utilization and Conservation of Forests' Communicated to Prof. Kerstein Wydra, Director, CeTSAF, for publication in proceedings of symposium on 'Ecosystem-based Management and Biodiversity Conservation' from December 05- 08, 2011 at Bogor Agriculture University, Bogor, Indonesia.

54. Swati Bisht, Ravi Kant and **Vineet Kumar** (2012) a-D-Glucosidase Inhibitory Activity of Polysaccharide Extracted from *Acacia tortilis* Plant Exudates. International Journal of Biological Macromolecules (communicated).

55. Swati Bisht, Ravi Kant and **Vineet Kumar**. Antidiabetic Activity of *Acacia tortilis* Polysaccharide on Streptozotocin-NAD Induced Type 2 Diabetes Mellitus in Albino Wistar Rats. Journal of Diabetes and Its Complications (communicated).

Polysaccharides based therapeutics: Structure and Derivatization

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drvineet@gmail.com

Glycotherapeutics is stimulated by the fact that a vast number of biological events are triggered, mediated or otherwise influenced by polysaccharides. They are effective information molecules on cell surfaces and code for vast information required for a wide array of biological recognition processes, such as bacterial and viral infection, cell adhesion, signal transduction, differentiation, development, regulation and many other intercellular communications. Changes in glycocalyx constituents are observed in cancer, metastasis, inflammation, and viral diseases. Capsular polysaccharides based Pneumococcal, Meningococcal, Typhoid Vi vaccines have revolutionized the therapy since many strains of the disease microbes have become resistant to existing drugs and therapy. Further, intense research work is being done for development of vaccine for Malaria, Leishmeniasis, Cancer, HIV, Pneumonia, Influenza, Anthrax, etc. It is being increasingly realized that saccharide-mediated recognition is a fascinating area for drug discovery.

The paper discusses simpler and efficient routes towards chemical modification of hyaluronic acid due to its remarkable physico-chemical characteristics and unique biological functions. HA is employed in a wide range of current and developing applications in rheumatology, ophthalmology, drug and gene delivery, wound healing and tissue engineering. The use of HA in some of these applications is limited due to its rapid degradation by *hyaluronidase* in the body, and thus difficult to process into biomaterials and as drug candidate. A number of significant modifications of HA (acrylation, crosslinking, esterification, glycopeptides) have been achieved using novel, facile, green and cost-effective routes for varied biomedical applications.

In the later part, isolation, purification, chromatographic analyses and chemical composition of novel and interesting plant polysaccharides viz. *Cassia tora* seed, *Dalbergia sissoo leaves, Tinospora cordifolia* stem will be discussed based on chemical and advanced spectroscopic methods. Enthused by the superior antidiabetic activity of polysaccharides of *Acacia tortilis* gum exudates, it has also been embarked to study its fine structure. The paper details chemical composition of the oligosaccharides and polysaccharide based on extensive separation and advanced spectroscopic analysis with a view to establish the fine structure of the novel bioactive polysaccharides.

REFERENCES

1. Gross, R and **Kumar, Vineet**. PCT/US07/63671 dated March 09, 2007 International Publication No: WO 2007/10678 A2 dated 20 September 2007. EP 2007758243 **Granted 30.12.2009** US No 12280187 (22.08.2008); AU No. 2007226690 (14.08.2008); CA 2647481 (11.09.2008); CN 200780009291.9 (16.09.2008); JP No 2009500563 (03.09.2008)
2. **Kumar, Vineet;** Rana V., and Soni, P.L. (2013). Phytochemical Analysis 24, 75-80.
3. Jindal M; Kumar, Vineet; Rana V; Tiwary A. K (2013). Carbohydrate Polymers (In press, accepted manuscript) http://dx.doi.org/10.1016/j.carbpol.2012.12.012
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Invited Lecturer-44D

Prof. Maheep Bhatnagar

Prof. Maheep Bhatnagar, Dean and Chairman Faculty of Science at M.L.Sukhadia University is a internatonally acclaimed neurobiologist, known for his extensive research contribution in the area of neurochemistry, aging, neurodegeneration and neuroprotection. He is expert of Light and electron microscopic immunocytochemistry and Neuonal Cell culture. His research in fluoride toxicity and plant derived antiulcer drugs has also been appreciated by the scientific community. His research is published in Brain research, Neurobiology and aging, Brain and Behaviour, Thorax, Regulatory peptides, Proceedings of New York academy of sciences, Cellular and molecular Biology, Phytotherapy Research, ethnopharmacology, Herbal pharmacotherapy etc. His work has been extensively cited by other researchers in their publications (Citation index more than 200 till 2007). Prof. Bhatnagar is also on editorial board of several International and national journals and is reviewer for Neurochemistry, Neurobiology, Pesticide Biology, J Alternative Medicine, Cell tissue research, Ind.J.Exp. Biology, Medical Science Monitor etc. Professor Bhatnagar has published approximately 89 research papers, 30 articles and reviews and contributed several chapters in books. He was Editorial Advisor with Prof Micheal Achner on Book entitled **Neurochemistry of metabolic diseases** – Lysosomal storage dieseaes, Phenylketonuria and Canavan disease published from USA. Professor Bhatnagar was President of the Indian Academy of Neurosciences (2004-05) and Society of Science and environment (2005-2006). He did postdoctoral at Royal Postgraduate medical School under guidance of Prof. Julia Polak, at Oregon Primate research center with Prof. Vaughn Critchlow. He served as Guest Scientist at Cellular and Mol. Neurobiology Div, Karolinska Institute. He was invited as Visiting Professor to Div. of Biotechnology, Shanxi University, China. He was Governors Nominee to Navsari Agri University, Gujrat. He is also recipient of Biotechnology award, CV Kapoor foundation distinguished teacher award, Bharat Jyoti award and Prof. D.M. Kar award. He is fellow of several societies viz, Fellow of World Congress of Cell and Molecular Biology (France), Royal Microscopical Scocity (UK); Zoological Society of London (UK) ; Indian Academy of Neuirosciences (India), National environmental science Academy, Society of Science and Environment and also life member of several societies. He has also served as advisor to NGO "SARITA" working in the tribal area for awareness generation on fluoride toxicity. He is Editor in Chief of a Peer reviewed Indexed journal " J. Herbal medicine and Toxicology.

BRIEF CV OF PROF. Dr. MAHEEP BHATNAGAR

Full name: Dr. MAHEEP BHATNAGAR

Present position: Dean and Chairman, Faculty of science And Professor and Head, Dept of Zoology

Course director- Microbiology

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Academic achievements:

Master of Science in Zoology from University of Udaipur, India
Ph.D. in Developmental Neurobiology from University of Udaipur, India
Diploma in Endocrine Pathology from Hammersmith Hospital, London
Diploma in Animal Medicine- Karolinska Institute, Sweden

Postdoctoral - Royal Postgraduate Medical school, Univ of London , London
Postdoctoral- Oregon Primate research Centre, Beaverton, Oregon, USA
Postdoctoral- Karolinska Institute, Stockholm , Sweden

Fellow of Word Congress of Cellular and Molecular Biology, Paris

Fellow of Indian Academy of Neurosciences, Allahabad, India.

Fellow National Environmental Science Academy, New Delhi

Fellow Society of Science and Environment, New Delhi.

Area of research interest:

1. **Neuroprotective effects of various compounds of natural origin.**
   (We are working on protective effects of RESVERATROL, *WITHANIA SOMNIFERA*, *ASPARAGUS RACEMOSUS*, *CANTELLA ASIATICA*)
2. **Protective effects of natural products on fluoride induced neurotoxicity**

Publication: Total publication 110

Articles: 20
Book Chapters: 10

Books-:10

Editorial assignments:

Chief Editor- Journal of Herbal Medicine and Toxicology, An Online and Print journal

Co-Editor- Journal Cell Tissue research, An Online and Print journal

Member editorial board- International Journal of Environmental Sciences
Journal of Neurobiology and behaviour
Phamacognosy Journal
Medical Science Monitor

Students obtained : Ph.D. 25

Students working for Ph.D : 06

Students did dessertation : 25

Mobile phone radiations (900MHz radiofrequency): Effects on structure and physiology of brain.

Maheep Bhatnagar

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ABSTRACT

The extensive use of mobile phone communication has raised public concerns about adverse health effects of radiofrequency (RF) electromagnetic fields (EMFs) in recent years. The topic of discussion is that whether regular use of mobile phone alters human health significantly. The effects of mobile phone radiations on behavior, biochemistry and histology of rat brain was studied because it is the most exposed part to mobile radiations and the central control system of the body. Male wistar rats (age one month) were exposed to 900 MHz radiowaves by means of Spice S-5110 handset @ 4 hours per day for 15 days. Thereafter, effect on anxiety, spatial learning and memory was studied using open field test, elevated plus maze, morris water maze and classic maze. Since oxidative stress is thought to be involved in radiation induced damage, biochemical tests have also been performed to estimate enzymatic and non enzymatic antioxidants. Finally, tissues were stained in cresyl violet to check the possibility of neurodegeneration. The results indicated a significant change in behavior of test animals as compared to controls with more anxiety and poor learning shown by exposed animals. Biochemical alterations were also seen as decrease

in activity of antioxidant enzymes and change in concentration of antioxidants. Lipid peroxidation had also increased in test rats. Histological examination showed neurodegeneration in hippocampus and cerebral cortex in response to mobile radiations. Thus our study demonstrates a pronounced effect of mobile radiations on the rat brain.

Award lectures

ISCB AWARD FOR EXCELLENCE 2013

Nanomaterials for societal applications

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Synthesis of nanomaterials with controlled size and shape is a challenge to materials community. In view of this, novel synthesis protocols have assumed a crucial importance. Of late, the soft chemical routes have gained an unprecedented significance. In my group, various nanomaterials for energy conversion, environmental and health related applications are being synthesized. The control of morphology is another important parameter for various applications. The emphasis of this talk will be on preparation of nanomaterials for applications in water remediation and drug delivery. Some typical results of defluoridation of drinking water and development of sensor for toxic metal ions detection will also be discussed. Another promising but currently under-explored area is the application of nanomaterial based sorbents for the chromatographic separation of radioisotopes for health applications. The development of nanomaterial based sorbents for radionuclide separation is a growing research area which requires collaborative efforts of material chemists, radiochemists, analytical chemists and radiopharmaceutical chemists. Development of various sorbent materials for the application in radiochemical generator (^{188}W-^{188}Re, ^{99}Mo-^{99m}Tc and ^{68}Ge-^{68}Ga) will also be elaborated. A NiS-PMMA based composite was prepared for the separation of ^{106}Ru, a radionuclide for ocular cancer treatment. Likewise, sorbents have been designed, using crystallographic concepts, for the uptake of ^{241}Am for the nuclear waste stream. Some of these results will also be discussed during this talk.

Acknowledgement: The Radiochemical generator part of this work was done in collaboration with Radiopharmaceuticals Division, BARC and the ^{106}Ru and ^{241}Am uptake work was done in collaboration with Nuclear Recycle Group, BARC. Their contribution is sincerely acknowledged.

ISCB Young Scientist award in the area of chemical sciences

Ionic Liquid Applications: Solvents, Reagents, Catalysts and Soluble Support

Anil Kumar

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Ionic liquids are fascinating materials for chemists with unique physiochemical properties and have numerous advantages over other liquids.[1] They have negligible vapour pressure and are miscible with water or organic solvents. In the last decade, functionalized ionic liquids (FILs) synthesized with properties for specific chemical tasks in mind have attracted attention of chemists. FILs are now used as alternative supported tools, scavengers, catalysts, and as well as reagents.[2] As a part of our research,[3] we became interested in applications of ionic liquid for various organic transformations. We have synthesized a novel ionic liquid functionalized with aldehyde group. This functionalized ionic liquid was used for ionic liquid-supported synthesis of amides and sulfonamides[4a] and as scavenger for primary amines in synthesis of secondary amines by reductive amination.[4b] An ionic liquid-supported sulfonyl azide was developed as an alternative diazotransfer reagent for active methylene compounds.[4c] Ionic liquid-supported sulfonyl hydrazine was used as 'catch and release' reagent in synthesis of 1,2,3-thiadiazoles and 1,2,3-selenadiazoles.[4d] The approach provides a way to synthesize organic molecules with simplified purification, requiring no chromatography during the synthesis or at the end of cleavage of the product from support. Details of different protocols developed using ionic liquids will be presented.

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Life time achievement award

NMR in Health Sciences: Diseases and Brain Function

C.L. Khetrapal

Centre of Biomedical Magnetic Resonance,Sanjay Gandhi Post Graduate Institute of Medical Sciences Campus, Lucknow

Rapid development of NMR techniques and technology during the past nearly seven decades from the discovery of the phenomenon have been responsible for the exponential growth in the applications of NMR as a noninvasive tool for studying anatomy, structure and *in vivo* metabolism. However, developments of innovative techniques for understanding human diseases and brain function at molecular level are still in infancy and hence promise a bright future for research.

Variations in metabolic profile resulting from disorders and clinical intervention at molecular level are more sensitive in identifying diseases in early stages and assessing the efficacy of the interventions. Due to direct societal relevance, many private public partnerships are being rapidly established particularly in the developed countries to exploit such developments. National and international efforts in this direction will be highlighted with specific examples. Specifically results on amyotrophic lateral sclerosis, obstructive jaundice and cholangitis, sub-clinical infections in open heart surgeries will be presented. For such studies results obtained from bio-fluids such as urine, serum, bile acids, and pericardial fluid which have very complex metabolic profiles with numerous structurally similar metabolites will be described. Specific metabolic signatures for different diseases from such investigations will be illustrated. The brain function and behavioral results based on the functional Magnetic Resonance Imaging studies with emphasis on the effect of positive thinking, meditation, *mantras, Yoga* and learning languages will be discussed.

Best thesis award in the area of Drug research

Author: Dr. Poongavanam Vasanthanathan (nobelvasanth@gmail.com),chris.oostenbrink@boku.ac.at

Name of supervisor(s): Prof. Flemming S Jørgensen, Prof. Chris Oostenbrink, Assoc. Prof Lars Olsen, and Prof. Nico PE Vermeulen

Cytochrome P450s (CYPs) form a superfamily of hemethiolate containing proteins, which play a crucial role in the biotransformation of xenobiotics, including most of the therapeutic drugs, environmental pollutants and endobiotics, such as steroids, bile acids, fatty acids, prostaglandins, and leukotrienes. In humans, CYPs contribute to 70-80% of the phase I metabolism of currently marketed drugs. CYP1A2 constitutes ~13% of the total P450 content in the liver and plays an important role in the metabolic clearance of more than 10% of currently marketed drugs. Moreover, it is inducible by polycyclic aromatic hydrocarbons (PAH) and heterocyclic amines, which are found in cigarette smoke and charred food. It can activate pro-carcinogens to carcinogens, and an over-expression of CYP1A2 has been linked to a high risk of various cancers, including breast and colon cancers. Therefore, an early prediction and rationalization of CYP1A2 mediated metabolism and identification of novel inhibitors are essential in order to improve the drug therapy effectively. There are many challenges in understanding action of CYP1A2, however, from pharmaceutical point of view, there are certain challenges considered to be very important, e.g., isoform selectivity, site of metabolism, virtual screening (identification of inhibitors/substrate), binding affinity and polymorphism. Although majority of the above mentioned challenges were addressed in the thesis, this presentation will briefly explain, how we have successfully used computational models for identification of potent CYP1A2 inhibitors.

Best thesis award in Biological Science

Talk Title: Protein Quality Control Mechanisms in Neurodegenerative Diseases

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ABSTRACT

Cells regularly synthesize new proteins. In cellular compartments, old or misfolded proteins are substituted by new peptides. Failure of protein quality control mechanism leads various human diseases. For efficient quality control system cell always try to refold protein prior to their degradation. Protein synthesis and its folding is the chief cellular quality control process that governs the long-term health of the cell. Protein-folding homoeostasis or proteostasis cellular process is maintained by two evolutionary conserved modulators: molecular chaperones dependent stress response and unfolded protein response (UPR). Eukaryotic, cytosolic chaperone machineries are organized into two separate but overlapping networks: Stress inducible chaperones (Hsp70 family members) are protein-folding molecular machineries which abundantly expressed in various cellular compartments, whereas ribosomal-associated chaperones facilitate co-translational folding of nascent polypeptide chains and cooperate with protein translation bio-machineries. Under normal conditions, the local cellular concentration of chaperones and their functional activity is reserve with substrates. It has been determined that acute environmental and physiological stress conditions perturb normal cellular functions and generate proteotoxicity. To restore this delicate equilibrium, instantly cellular chaperones up-regulate their local abundance, apparent capacity and improve appointment of client proteins. However in protein homeostasis the precise functions of ribosomal-associated chaperones are unknown. Still it is not clear that how cellular early protection mechanism works against aggregation mediated proteotoxicity under various stress conditions? A better understanding of molecular chaperones and E3 ubiquitin ligases mediated deregulation contributes in the aggregation dependent proteotoxicity and progression of aggregation-associated human diseases.

ORAL

O-1

An organocatalytic direct Mannich–cyclization cascade as [3+2] annulation: Asymmetric synthesis of 2,3-substituted pyrrolidines

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Organocatalysis, known to mimic the characteristic of enzymes and biomolecules, has matured enough to be considered now as *'third pillar of asymmetric catalysis'*, since its renaissance with the beginning of this century.[1] However, direct amine catalysis *via* enamine and iminium-ion intermediates has now emerge as pathfinder for the modern chemists, to design an unambiguous products in a simple catalytic one pot operation.

The [3+2] cycloaddition of azomethine ylide with activated olefin is the most effective method known for the asymmetric synthesis of pyrrolidines.[2] On the other hand, the complementary [3+2] cycloaddition of suitable all-carbon 1,3-dipoles to imines have not been studied extensively, because of the unavailability of suitable 1,3-dipoles and low reactivity of imines. In the continuation of our interests,[3] we developed a simple and highly stereoselective method for substituted pyrrolidines from readily available precursors like; *N*-PMP aldimines and succinaldehyde as new 1,3-carbon dipole.[3a] The present one-pot protocol involves the L-proline catalyzed direct Mannich reaction and reductive cyclization sequence as formal [3+2] cycloaddition under mild condition, affords a wide access to *trans*-2,3-substituted pyrrolidines

Details of the concept, design and synthetic strategy will be presented here.

Scheme 1:

References:

(1) (a) K. Mikami, M. Lautens, *New Frontiers in Asymmetric Catalysis*; Wiley-Interscience: Hoboken, NJ, **2007**; (b) P. I. Dalko, *Enantioselective Organocatalysis*; Wiley-VCH: Weinheim, **2007;**

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O-2

Oxidative Aminocarbonylation of Terminal Alkynes for the Synthesis of Alk-2-ynamides by Using Palladium-on-Carbon as Efficient, Heterogeneous, Phosphine-Free, and Reusable Catalyst

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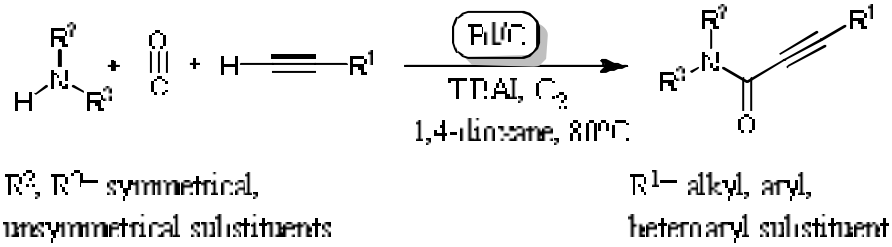
The alk-2-ynamides (*a,ß*-alkynylamides) are important building blocks in the synthesis of various heterocyclic compounds and biologically active molecules. They exhibit excellent affinity for the mGluR5 receptor and antifilarial activity. In context, Gabriele *et al*. reported a direct oxidative aminocarbonylation for the synthesis of *a,ß*-alkynylamides from alk-1-ynes and secondary amines by using PdI_2 and KI as a catalytic system in the presence of a CO/air mixture (20 atm) at 100 °C for 24 h. This seminal work was then followed by a report from Yamamoto *et al*. on using homogeneous $PdCl_2/PPh_3$ as a catalytic system for the direct oxidative aminocarbonylation using carbon monoxide/ oxygen (CO/O_2) in basic conditions with NaOAc as base. However reported methods suffer from one or mo re drawbacks.



Scheme 1: Oxidative aminocarbonylation of alk-1-ynes for synthesis of alk-2-ynamides.

In this regards oxidative aminocarbonylation of alk-1-ynes with variety of secondary amines under low pressure of carbon monoxide/oxygen (5/1 atm) was investigated by using palladium-on-carbon catalyst (Scheme 1). The catalytic system represents efficient, heterogeneous and phosphine-free approach for the synthesis of wide variety *a,ß*-alkynylamides. The developed protocol furnishes good to excellent yield of desired products within short reaction time. Present methodology circumvents the use of the phosphine ligands, bases and also solves the basic problem of palladium catalyst recovery. The catalyst exhibited remarkable activity and was effectively recycled for four consecutive cycles.

REFRENCES

1) B Gabriele, G Salerno, L Veltri, M Costa, J. Organomet. Chem. 622, 2001, 84.
2) S Gadge, M Khedkar, S Lanke and B.Bhanage, Adv. Synth. Catal. 354, 2012, 2049.

O-3

Selective and efficient synthesis of decahedral palladiumnanoparticles and its catalytic application for Suzuki coupling reaction

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A convenient, mild and cost-effective synthesis of decahedral palladium nanoparticles by exposing aqueous $PdCl_2$ solution to the sunlight in the presence of citric acid as a reducing agent and PVP as a capping agent was reported. The obtained nanoparticles were thoroughly characterized by using techniques like TEM, SAED, FEG-SEM, XRD and EDAX. It was observed that upto 70% of the palladium nanoparticles have decahedron shape. The citric acid helps in shapes selective synthesis, whereas concentrated solar energy supplies duel energy which helps to speed up the reduction process. The aqueous reaction mixture of palladium nanoparticles was directly employed for the Suzuki coupling reaction and hence centrifuging efforts and cost of reagents required for the isolation of nanoparticles were avoided. The synthesized nanoparticles demonstrated excellent catalytic activity in Suzuki coupling reaction of aryl halides with phenyl boronic acid under mild reaction conditions. The methodology is applicable to diverse substrates providing good to excellent yields of desired products. Notably, the obtained yields with lowest catalytic loading resulting in highest TOF (0.05 mol% catalyst loading and

TOF of 1960 h^{-1}) were among the best ever reported for the Suzuki coupling reaction. In addition, the catalyst could be reused for three more consecutive recycles. The effectiveness of present new protocol for the PdNPs synthesis was also compared with PdNPs prepared using conventional heating method.

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[2] A Patil, D Patil and B Bhanage, j mol cat:A (Just Accepted)

O-4

A novel method for the synthesis of 5-subtituted 1*H*-tetrazole from Oxime and Sodium Azide

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Tetrazoles are heterocyclic compounds having five membered ring containing one carbon and four nitrogen atoms. Such heterocyclic systems are not found in nature. Tetrazole have a wide range of applications in pharmaceutical chemistry [1] especially in drugs in isosteric replacement of carboxylic acid moiety [2]. Biphenyl tetrazoles are used for the synthesis of sartan family drugs [3]. Recently tetrazole moieties were widely used for binding aryl thiotetrazolylacetanilides with HIV-1 reverse transcriptase.

Herein we report the simple and efficient protocol for the synthesis of 5-substituted 1*H*-tetrazoles from various oximes and sodium azide (NaN_3) by using copper acetate as a catalyst. The developed protocol is novel, greener and atom economical. Replacement of toxic nitriles precursors by oximes is the novelty of this protocol. Higher yields, simple work-up procedure, easily available and cheaper catalyst are the added advantages of this protocol. Hence, replacement of nitriles and use of cheaper as well as easily available catalyst makes this protocol feasible and economically attractive [4].

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O-5

Synthesis And Evaluation Of Antioxidant Activities Of Some New 3-Substituted-2-Oxindole Derivatives

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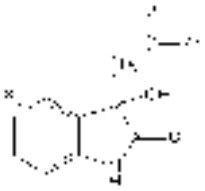
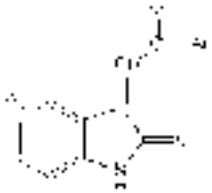
Indolic compounds are a broad family of substances present in microorganisms, plants and animals. Considering plant hormone, indole-3-acetic acid, and the animal hormone, melatonin, an important characteristic of indolic compounds is their usefulness as chemical preventive agents against diseases such as cancer, oxidative stress. Gacche et al. [1] 3-substituted-2-oxindoles has been recently recognized as a privileged scaffold displaying potent antioxidant, anticancer, anti HIV, neuroprotective activities. Alves et al. [2]

For this reason, in the present study, a series of new 1,3-dihydro-3-hydroxy-3-(2-phenyl-2-oxoethyl)-2H-indol-2-ones (Ia-g) and 1,3-dihydro-3-(2-phenyl-2-oxoethylidene)-2H-indol-2-ones (IIa-g) were synthesized by Knoevenagel condensation of 5-substituted indole-2,3-diones (isatins) with various acetophenones. Popp et al. [3] The structures of the products were characterized by their physical data, elemental, IR, ^{1}H NMR, ^{13}C NMR and mass spectral analyses. *In vitro* antioxidant

activities of the synthesized compounds were determined by 2, 2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging assay, Brand-Williams et al. [4] total antioxidant capacity, Prieto et al.[5] and ferric reducing antioxidant power method. Oyaizu et al. [6] The synthesized compounds showed moderate to good antioxidant activities as compared with the standard, ascorbic acid. 3-Hydroxy-3-substituted oxindoles (Ia-g), showed concentration dependent antioxidant activity in concentration range varying from 10-500 µg/ml with 5-fluoro and 5-methyl analogues showing maximum activity by all the three methods. For 3-aroyl methylene indol-2-ones (IIa-g), most compounds with halogen substitution at position 5 of isatin ring exhibited good antioxidant activity within concentration range from 5-100 µg/ml and the maximum activity was observed at concentrations 20 and 25 µg/ml. Thus, our study provides evidence that some newly synthesized isatin derivatives had significant antioxidant activity at low concentrations.



(Ia-g)



(IIa-g)

X= 5-H, 5-F, 5-Cl, 5-Br, 5-CH_3

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O-6

PHARMACOPHORE MODELING, 3D QSAR, VIRTUAL SCREENING, DOCKING AND *IN SILICO* PHARMACOKINETIC AND TOXICITIES PREDICTION STUDIES OF PROTEIN KINASE B (AKT *β*) INHIBITORS

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Protein kinase B (Akt) is a key mediator of proliferation and survival pathways that are critical for cancer growth. Therefore, inhibitors of PKB could be useful for the treatment of tumours. Herein, we describe pharmacophore-based 3D QSAR (CoMFA and CoMSIA) and virtual screening combined with docking study as a rational strategy for identification of novel hits or leads. A total number of 12 PKB/Akt *β* inhibitors were used to generate pharmacophore models applying DISCOtech and GASP. The best ranked model was used for the alignment of the compounds in 3D QSAR study. A data set of 73 compounds consisted of 4-amino-1-(7H-pyrrolo[2,3-d]pyrimidin-4-yl)piperidine-4-carboxamides [1], 4-(4-aminopiperidin-1-yl)-7*H*-pyrrolo[2,3-*d*]pyrimidines [2] and 6-phenylpurine [3] was used for the generation of QSAR models. Pharmacophore-based virtual screening was performed to search NCI database. A total of 53 compounds were identified as good PKB/Akt *β* inhibitors. Among these molecules, those who have a Qfit value more than 78% were docked on PKB to further explore the binding mode of these compounds. Finally *In silico* pharmacokinetic and toxicities were predicted for best docked molecules. The hits reported here showed good potential to be PKB inhibitors.

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O-7

DISCOVERY OF HIV-I INTEGRASE INHIBITORS: PHARMACOPHORE MAPPING, DATABASE SEARCHING, MOLECULAR DOCKING, SYNTHESIS AND *IN SILICO* PHARMACOKINETIC & TOXICITIES PREDICTION.

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Integrase inhibitors, class of anti-retroviral drug, block the action of integrase-a viral enzyme that inserts the viral genome into the DNA of the host cell. Here, we used CADD approaches to design potent HIV-I integrase inhibitors using SYBYL X1.2 software [1]. Twenty molecules from previously published research articles were selected for pharmacophore mapping using DISCOtech and refinement using GASP. Ten pharmacophore hypotheses were generated and model 1 was considered the best model as it has highest fitness score compared to all other models. The best pharmacophore hypothesis contained 4 features including 2 donor sites, 1 acceptor atom and 1 hydrophobic region. Best model 1 generated was used as query for virtual screening from NCI and Maybridge database. A total number of 17930 molecules were obtained after Lipinski filtering. From this results, 30 molecules bearing pteridine core structure were designed by knowledge based structure activity relationship study and were docked on HIV-I integrase enzyme [PDB: 3L2T] [2] to predict the binding orientation of drug candidates to their protein target. From this, six molecules showing comparative score with standard drugs raltigravir and elvitegravir were synthesized. It also revealed that these compounds formed hydrogen bonds with two conserved region amino acids viz. Asn-155 and Lys-159. Six different 2-mercapto-6,7-substitutedpteridin-4-ol derivatives were synthesized [3,4] and characterized by FTIR, ^{1}H NMR and Mass. *In silico* pharmacokinetic and toxicity studies were predicted for synthesized molecules using OSIRIS property explorer [5]. The compounds reported here showed good potential to be HIV-I integrase inhibitors.

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O-8

Benzotriazole Mediated Solution Phase Syntheses of *N*-protected Peptides, Hybrid peptides and their Conjugates

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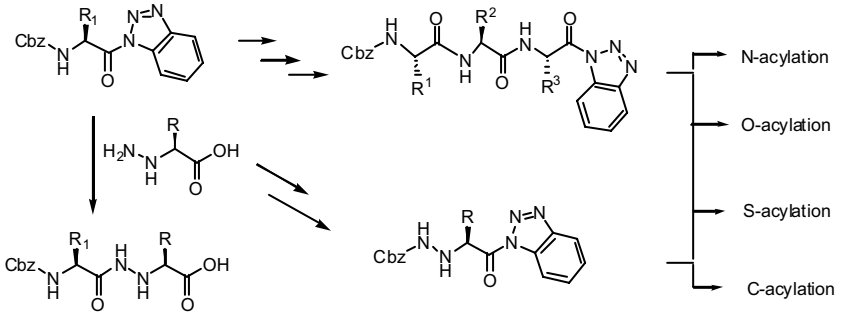
Peptides and their derivatives such as hormones, neurotransmitters and neuromodulators act as signal molecules in diverse biological and medicinal applications and thus have attracted considerable synthetic attention. The replacement of one or more *a*-amino acid by *ß*-amino acid units is a well-known technique in the search for pharmacologically active peptidomimetics. Hydrazino peptides, *i.e.*, peptide analogues in which one (or more) peptidic bond(s) [-HN-CO-CH(R)-] are replaced by one (or more) hydrazidic bond(s) [HN-NH-CH(R)-]. Vitamin B6 antagonist (Linatine) and antibiotic (Negamycin) are naturally occurring peptides containing *a*-hydrazino acid moiety.

Katritzky group have extensively utilized different *N*-acylbenzotriazoles for *N*-, *C*-, *O*- and *S*-acylations [1] and used *N*-protected aminoacylbenzotriazole for Solid Phase Peptide Syntheses up to six amino acids and solution phase synthesis of dipeptides. [2] Herein, we present the extension of that methodology for the convenient and efficient formation of Cbz-protected tri- and tetra-peptide conjugates with sugars, steroids, terpenes, and heterocyclic nuclei of biological importance. Also, a novel pathway to synthesize chiraly pure *a*-hydrazino acids and their solution phase conversion into both chiraly pure *a*-hydrazino hybrid dipeptides and *a*-hydrazino acyl conjugates by reacting with *N*-, *O*-, *S*-, *C*-nucleophiles. The detailed work and methodology will be discussed in the conference.



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O-9

Novel 4-Substituted 2-Dimethylaminotetralins: Synthesis and Binding Affinity at Serotonin 5-HT_2-type G Protein-Coupled Receptors with *In Silico* Docking Studies

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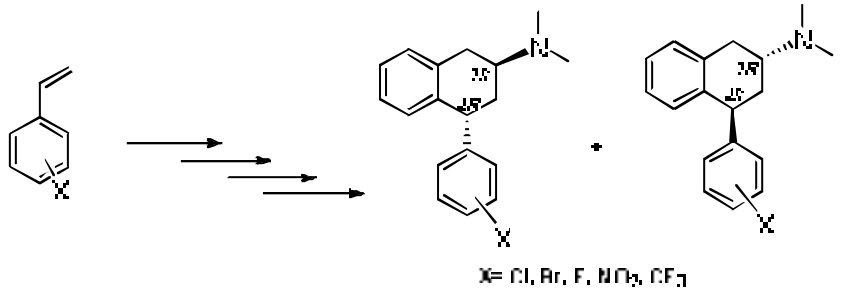
Activation of the brain serotonin (5-hydroxytryptamine, 5-HT) 5-HT_{2C} G protein-coupled receptor (GPCR) may be pharmacotherapeutic for neuropsychiatric disorders and obesity, whereas, activation of 5-HT_{2A} and 5-HT_{2B} GPCRs is associated with hallucinogenic and cardiopulmonary toxic effects, respectively. Sequence identity among the 5-HT_2 GPCRs is 75%, thus, precise molecular targeting is required. Based on the lead asymmetric *ß*-aminotetralin, (–)-(2*S*, 4*R*)-*trans*-4-phenyl-*N,N*-dimethyl-2-aminotetralin (PAT), that demonstrates antipsychotic efficacy without weight-gain after peripheral administration [1,2], this study used computational chemistry and molecular modeling studies to design 5-HT_{2C}-specific agonists. Of the 24 analogs synthesized and reported here, thus far, the (+)- and (–)-*trans* enantiomers of 4-(4'-chlorophenyl)-*N,N*-dimethyl-2-aminotetralin (*p*-Cl-PAT) were demonstrated to be 5-HT_{2C} receptor agonists with 5-$HT_{2A/2B}$ antagonist activity, and, were orally active in rodent models of schizophrenia and binge-eating, suggesting, potential as antipsychotic drugs without weight gain liability.

A series of *trans* 2', 3', and 4'-substituted (Cl, Br, F, NO_2, CF_3) PATs were synthesized starting from the corresponding styrene derivatives and trifluoroacetyl phenylacetyl anhydride *via* cascade Friedel–Crafts cyclic-acylalkylation, enolization, and O-acylation. [3] After reduction, tosylation and amination, the racemic products were obtained, which were separated using chiral stationary-phase preparative HPLC. The analogs were assessed for binding and function at human cloned 5-HT_2 receptors. The *p*-Cl-PAT enantiomers were administered orally to mice and found to negatively modulate locomotor behaviors in 3 different models predictive of antipsychotic efficacy, and, also were active to reduce food consumption in a binge-eating model. The detailed work and methodology will be presented in the conference.



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O-10

Nanotechnology and Medical Science: Challenges Ahead

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One nanometer (nm) is one billionth, or 10^{-9} of a meter. Materials reduced to the nano scale can suddenly show very different properties compared to what they exhibit on a macroscale, enabling unique applications. For instance, opaque substances become transparent (copper); inert materials become catalysts (platinum); stable materials turn combustible (aluminum); solids turn into liquids at room temperature (gold); insulators become conductors (silicon). Materials such as gold which is chemically inert at normal scales, can serve as a potent chemical catalystat at nanoscales. Nanotechnology matters because familiar materials begin to develop odd properties when they are of nano size. Tear a piece of aluminium into tiny strips and it will still behave like aluminum. But keep chopping them a smaller and at some point 20-30 nanometer pieces can explode. (Nanoaluminium may be used as rocket fuel).

Nanotechnology could prove to be a "transformative" technology comparable in its impact to the steam engine in the 18th century, electricity in the 20th century, and the Internet in contemporary society. Nanotechnology is a field of applied science and technology covering a broad range of topics. The main unifying theme is the control of matter on a scale below 100 nanometers, as well as the fabrication of devices on this same length scale. Richard Feynman described the concept of 'building machines" atom by atom in his talk titled "There is plenty of room at the bottom". **Top 10 use of nanotechnology include energy, water treatment, diagnosis of diseases, drug delivery, air pollution, construction material, health monitoring, pest control, agriculture and food processing.** Microscopes have offered scientists a window inside cells. Yet, what scientists have not been able to do is to answer questions such as, "How many cells are involved in cancer?" "How big is the cancer?" and "How fast a drug can be delivered at the exact place". The availability of innovative, body-friendly nanotools will help scientists how to build synthetic biological devices, such as miniature, implantable pumps for drug delivery or tiny sensors to scan presence of infectious agents or metabolic imbalances that could spell trouble for the body. In the treatment of brain tumour, laser guided smart bombs are used. Researcher at *University of Michigan* announced the testing of a drug delivery system that involves drug-toting nano particles and a guided peptide called F3. *PHOTOFRIN* a pharmaceutical which is photodynamic that means it can be activated by laser after it has entered in the blood stream to target cancerous cells of esophagus, bladder, skin and brain. In energy area also nanotechnology can play a vital role. Lighting alone accounts for about 8% of total energy consumption in Germany. The development of energy-saving lighting is therefore particularly important. Traditional light bulbs have an efficiency of only 5%. However, their light is similar to the light of the sun, which we perceive as pleasant. Modern low-energy bulbs have good efficiency, but at the same time their light is unpleasant for human eyes and they have a large-volume form. The light yield of semiconductors can now be increased drastically by using nanotechnology. Light is to be produced efficiently and in a pleasant colour from semiconductor material - similar to computer chips.

What is most important today is that people are not aware of the promises nanotechnology holds for the future especially for a country like India and other developing countries. Author who has started a novel concept of science communication called scientoon (a new class of cartoons based on science) and subsequently a new science called Scientoonics, will use this science to create awareness about Nanotechnology as what enormous future nanotechnology holds specially in the area of medical and pharmaceutical sciences.

O-11

Spontaneous Self-assembly of Renewable Nano-sized Triterpenoids: Formation of Fibers, Spheres and Vesicles

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Plant metabolites are the most significant source of *renewable* chemical feedstocks for a sustainable future. Among various plant secondary metabolites, triterpenoids are a large and structurally diverse C30 subset of the major component terpenoids. Computations carried out by us on sixty representative naturally occurring triterpenoids have established that *all the triterpenoids are nanometer long* having varied rigid and flexible lengths [1].

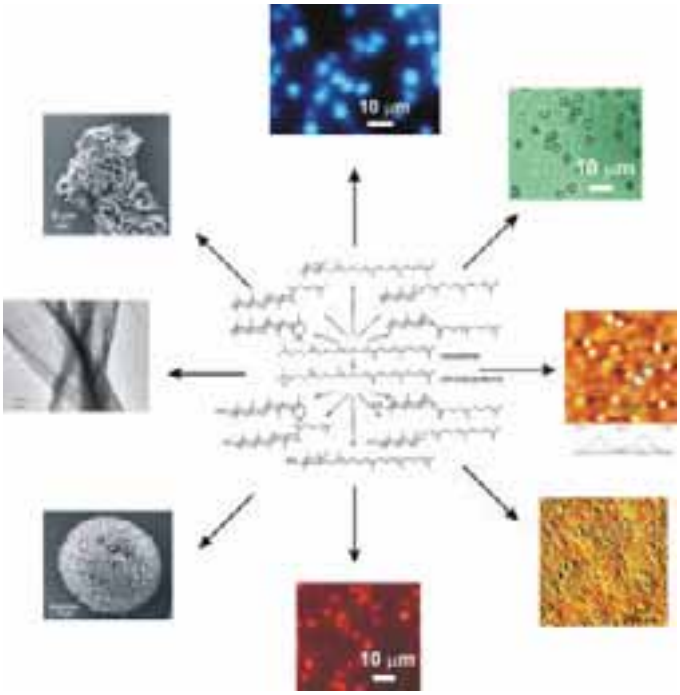

Figure 1: Schematic representation of the formation of nano-architectures from triterpenoids.

We have been successful in isolating several triterpenoids from different plants and initiated a long term project to utilize such *renewable nanos* in the design of nano-architectures and functional nano-materials. Detailed self-assembly studies revealed that these nano-sized triterpenoids and their derivatives self-assembled in different liquids at low concentrations affording self-assembled nano-arthitechtures such as helical nano-fibers, nano-vesicles, nano-spheres, etc. [2,3,4].

The alkyl chained esters of the nano-sized chiral arjunolic acid **1** could immobilize various organic solvents at low concentrations [5]. The molecules self-assembled in organic media to form nano-sized vesicles and helical nano-fibers with concomitant hardening of the media (Figure 1). The melting of a soft-solid material could be observed visually by concomitant color change [6,7]. Recent results from our laboratory will be presented in the perspective of Green, Renewable and Nanos.

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O-12

Synthesis, antitubercular evaluation and Recursive partitioning analysis of some Imidazo[1,2-a]pyridine derivatives

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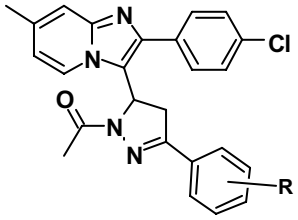
Imidazopyrimidine represent important building blocks in both natural and synthetic bioactive compounds which have shown to possess diverse therapeutic activities[1,2].The nature and the position of substituent's on the pyridine moiety influence these activity[3].Keeping this in mind, we have contemplated on the synthesis of pyrazolo derivatives bearing a imidazo[1,2-a]pyridine moiety. A series of pyrazole clubbed imidazo[1,2-a]pyridine have been synthesized by using the cyclo-condensation reaction of chalcones with hydrazine hydrate and their ability to inhibit growth of Mycobacterium tuberculosis in vitro have been determined.

The results show that compounds ss-12 exhibited excellent anti-tubercular activity with IC-90 6.67 µg/ml where as other compounds exhibited moderate to good anti-tubercular activity. A classification SAR model was developed using recursive partitioning (RP) approach to identify the structural characteristics structural characteristics that could be tuned to improve activity. The decision tree derived from the RP model could identify and interpret the descriptors that discriminate imidazo[1,2-a]pyridine analogues.



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O-12A

Design and Synthesis ofFuropyrazine Scaffold asConformationally Restricted Dipeptidomimetic

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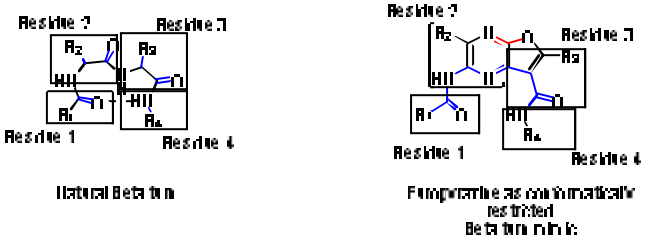
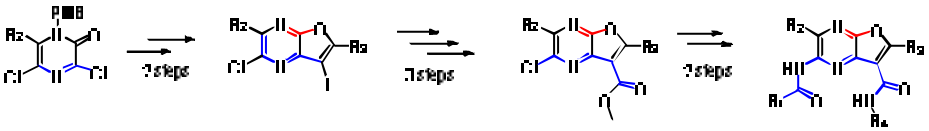
Proteins and peptides are interesting targets for drug development. However, the use of proteins and peptides as drugs is limited due to their poor bioavailability, immunogenicity and unfavourable pharmacokinetics.[1]Mimicking these specific secondary structures of the protein molecules such as a-helix, ß-sheet, ß-turn and loops, that constitute the bioactive surfaces involved in the receptor-ligand interaction, is a widely used approach in drug-development.[2] Non peptidic molecules which can mimic the secondary structures of proteins are therefore attractive compounds for drug development.[3] Scaffolds possessing these characteristics have a high possibility of becoming a "privileged scaffold".

Our previous research work involves synthesis of various heterocyclic molecules with an aim of getting lead candidates for various medicinal applications and has been well documented in literature.[4] Herein, an efficient synthetic approach to a furopyrazine scaffold with four points of diversity, startingfrom 2(1H)-pyrazinones, with dipeptomimetic properties, is presented.[5] The furopyrazine scaffold was further functionalized with an amino- and a carboxy-terminusresulting in a conformationally restricted dipeptidomimetic scaffold. The carboxy-terminus was introducedvia a chemoselectivevinylation of the 7-position followed by oxidative cleavage, while theamino-terminus was obtained via BuchwaldeHartwigamidation of the 2-position of the scaffold (**Scheme 1**). Theversatility of the synthetic method was demonstrated by the synthesis of a small library of diverselysubstituted furopyrazines having various amino acid side chains on the four points of diversity. Evaluationwith an X-ray structure of the scaffold and computational analysis supports the exploitation ofthe furopyrazine scaffold as a restricted dipeptide mimic, which can mimic the two central residues ofa ß-turn.





Scheme1

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O-13

Patent Trends in last 5 years in the area Life Style Disease

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The challenge we face today is not of information access, but of information utilization for best of our benefits. We would present a case-study on the Patent trends published in last five years in the area of Lifestyle related Diseases. This would be accomplished by analysing, datamining and finding correlations between published Patents vis -à-vis the scientific information disclosed. The benefit of such Patent trends and Research Landscapes can make research / patent decisions faster and more productive. This paper would also discuss India vis -à-vis Global Patent Trends.

We would quickly analyze thousands of published patents to find out :-

- Patents Trends - Types of Lifestyle related diseases, Patent Countries, Key Researches, Key Organisations/Institutes
- Patent landscape - determine who, what, where, when, and why
- Find out "White spaces" in the research and patents
- Locate organisations/institutes involved in similar research globally and explore collaboration opportunities
- Discover new arenas of research

Additionally, we would present a case study and analyse the compounds disclosed or claimed to treat one of the life style diseases with respect to core active moieties, correlation between whihc Organisations are working on what kinds of moeities etc. Finally, we would select one of the common core moieties and datamine published patents further to locate any other bioactivities that may have been reported elsewhere.

O-14

Pharmacological activity of the active constituents isolated from *some medicinal plants*

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Obtaining the drug from plants have been a traditional way in the Indian system of medicine and will remain the basis of the modern medicine. Broadly, the process of the discovery of drugs from plants consist of the discovery of the lead molecule (s) followed by its efficacy in biological system, animal toxicity, human clinical testing consisting of Phase 1, 2 and 3 and finally approval from the FDA. Recent, breakthrough in the discovery of the pharmacologically active constituents/lead molecules from traditional medicinal plants were the isolation of the texol from *Taxus brevifolia* for the treatment of cancer and artemisinin isolated from *Artemisia annua* for the treatment of drug resistant malaria. In the view importance of medicinal

plants in the area of drug discovery research and continuation of our effort to isolate and identify the chemical constituents and active principles from traditional medicinal plants [1-4], recently, we have isolated some active principles from medicinal plants by bioassay guided fractionations. In this presentation isolation procedure and structural elucidation and biological activity of the active principles isolated in our laboratories will be discussed in detail.

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O-15

Metabolic profiling of fruits of different chemotypes of *Withania somnifera* (L) Dunal using GC-MS and NMR spectroscopy

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Withania somnifera (L.) Dunal commonly known as Ashwagandha, is one of the most valued medicinal plants with a number of pharmaceutical and nutraceutical applications. The plant is recommended in many Ayurvedic recipes and has been employed in the treatment of neurological disorders, geriatric debilities, arthritis and stress- and behavior related problems Gupta & Rana [1]. Withanamides present in the fruits of this species have been reported to have efficient lipid peroxidation inhibitory activity and potential to prevent progression of Alzheimer's disorders Jayaprakasam et al. [2, 3]. Metabolic profiling was performed by GC-MS and NMR spectroscopy on the fruits obtained from four chemotypes of *W. somnifera*. A combination of ^{1}H NMR spectroscopy and GC-MS identified eighty two chemically diverse metabolites consisting of organic acids, fatty acids, aliphatic and aromatic amino acids, polyols, sugars, sterols, tocopherols, phenolic acid and withanamides from the fruits of *W. somnifera.* Eighty two primary and secondary metabolites from the fruits of *W. somnifera* were identified using NMR spectroscopy and GC-MS. Squalene and tocopherols are the most potent naturally occurring compounds with antioxidant properties were identified by us for the first time in the fruits of *W. somnifera*. Application of PCA and ^{1}H NMR spectroscopy on the quantified metabolites revealed a clear separation between chemotypes of primary and secondary metabolites. The qualitative and quantitative variations in the metabolites among different chemotypes of the fruits of *W. somnifera* suggest that specific chemotypes can be used for obtaining substantial amounts of bioactive ingredients for getting the desired pharmacological and nutraceutical activities.

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O-16

Stereocontrolled oxidative additions upon 1,4-dihydropyridines: Synthesis of hexahydrofuro[2,3-b]pyridine derivatives

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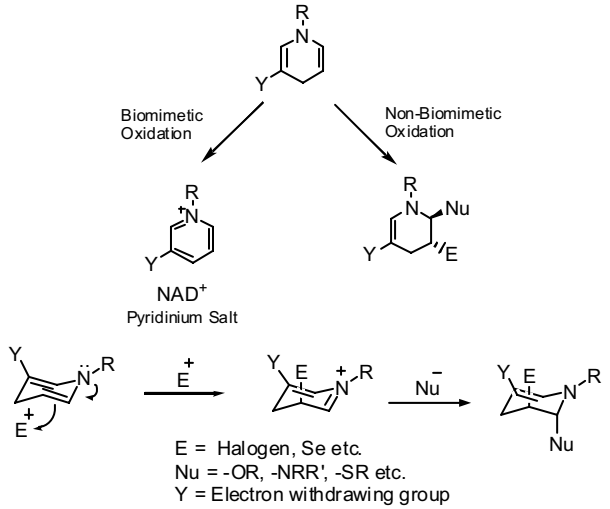
[b]Department of Chemistry, University of Delhi, India

Continuing our research on the development of new transformations of 1,4-dihydropyridines, we have recently described some 'non-biomimetic' oxidations of these compounds, in which the normal production of the corresponding pyridinium salt is avoided **[1]**. The methodology represents a new synthetic entry to a wide range of functionalized tetrahydropyridines stereoselectively as potential precursors of bioactive or natural products such as azasugars. This methodology also affords bicyclic heterocyclic systems **[2-3]** of biological importance. Electrophilic interaction of halogen with *N*-alkyl-1,4-dihydropyridines followed by the reaction of iminium salt with nucleophile allyl alcohols, propargyl alcohol, 2-butyn-1-ol and 3-butyn-1-ol stereoselectively lead to the functionalized tetrahydropyridines which are converted into corresponding hexahydrofuro[2,3-b]pyridine derivatives in satisfactory yields by free radical cyclisation reaction.



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O-17

Engineering Techniques for QSAR of Peptides

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Peptides and proteins are of prime essence in all living systems.Peptides are considered as drugs of choice becauseof their high potency (low dose), specificity, and selectivity(reduced side effects). Optimization of peptidesis a cumbersome process and the complexity increaseswith the length of the peptide sequence. Simple experimentalmethods used for checking the effect of an alteration of an amino acid (mutation) include a systematic amino acid. However a complete optimizationcan never be achieved by such methods. Use of computational approaches such as QSAR and simulationmethods in complement to the experimental techniques gives user an advantage to make the process of peptide optimizationa tractable task.

Peptide QSAR techniques were developed at the lab to solve and overcome problems related to design of peptide ligands:

Descriptor-based and Binary QSAR was developed to understand and identify the specific nature and type of amino acids at the different positions in a given peptide sequence that modulate biological activity using the classical Hansch and Free-Wilson approaches. These approaches werevalidated on peptides that bind to the Major Histocompatibility Complex (MHC).

HomoSARwas developed to reduce the uncertainties associated with the 3D-alignment of peptides, which is acrucial step in standard 3D-QSAR studies like CoMFA and CoMSIA. This approach is based on use of comparative protein modeling principles in tandem with standard 2D-QSAR technique. The positional similarities or dissimilarities serve as the parameter to evaluate the nature and position of amino acids desirous in the peptide sequence. This approach was validated on peptide datasets that belong to Major Histocompatibility Complex (MHC), ACE inhibitory peptides, hAmiphiphysin-1 and CAMEL peptides.

ensemble QSAR (eQSAR) approach was designed to improvise the '*one chemical–one structure–one parameter value*' dogma where propertiesrelated to a single molecular conformation are correlated to the biological activity while all other structures are ignored (a drawback in QSAR analysis). *e*QSARuses the properties *(physicochemical descriptor matrices)* generated for an *ensemble* of molecular conformations to understand the variation in the biological activity in a dataset. The method was validated on datasets viz. bradykinin-potentiatingpentapeptides, bitter tastingdipeptides and the ACE inhibitory tripeptides.

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O-18

New Rearrangements of Semiaminals of Natural Origin

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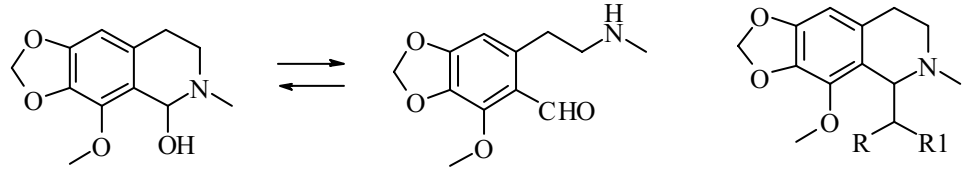
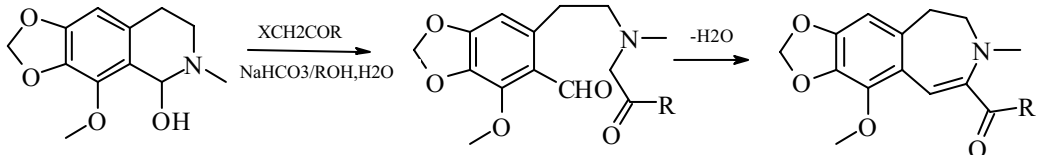
Alkaloid cotarnine **1** [1-3] a pseudobase of isoquiniline group, is an interesting object of study due to its multi-faceted reactivity, stemming from ring-chain tautomerism 1⇆2. Earlier we reported a series of studies on the interaction of cotarnine with CH-acids leading to compounds of type **3** [4-9].



1 **2** **3**

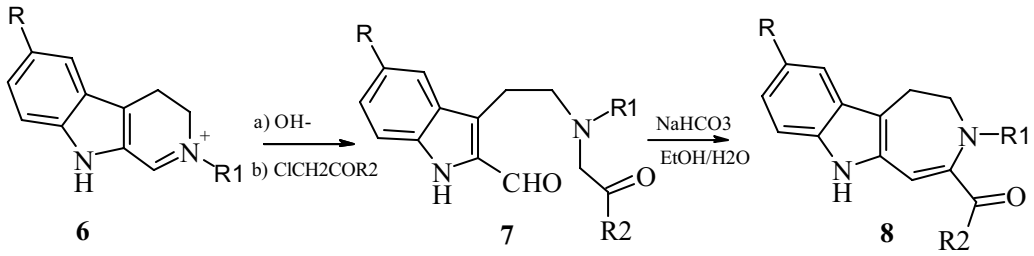
Our recent studies have shown that the interaction of cotarnine with a-halogen ketones (upon boiling the components in an aqueous-alcoholic medium in the presence of NaHCO3 for 10-30 minutes) leads to a rearrangement which results in the formation of 3-benzazepine derivatives **5** with yields of up to 90%.:



1 **4** **5**

R= Alk, Ar, Het; X=Cl, Br

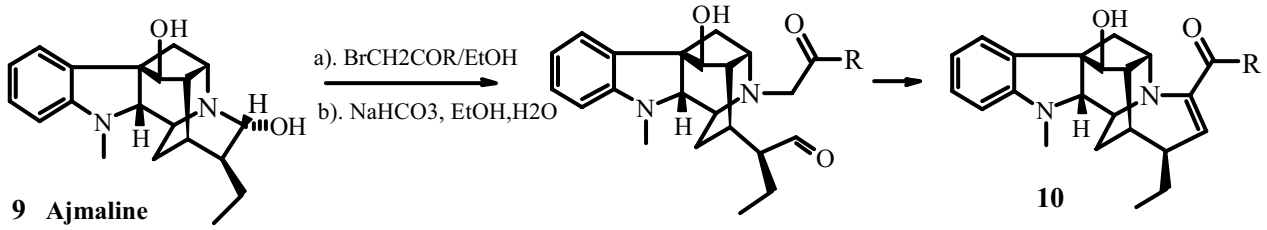
In the course of the study on the discovered recyclization of natural semiaminals, we used 2-N-alkyl-3,4-dihydrocarboline iodides **6,** which produced azepine[4,5-*b*]indoles **8** through intramolecular cyclization of the intermediates **7** (upon boiling with NaHCO3 in aqueous ethanol) with a yield of 40-52%(R=CH3), 50-64% (R=Ph) and 35-38% (R=Ind-3)**:**



6 **7** **8**

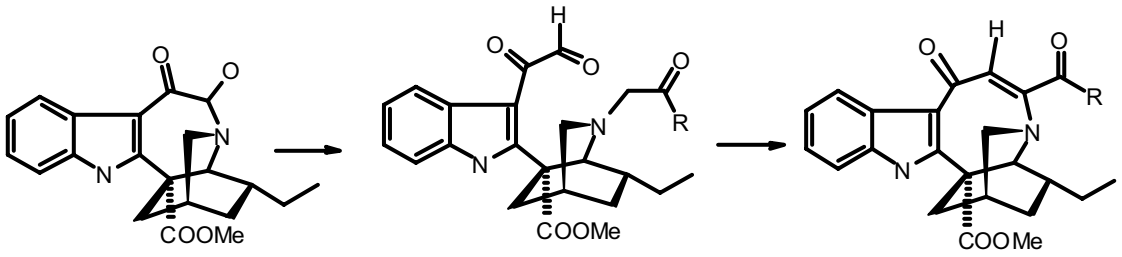
R=H, Alk, OCH3; R1= CH3, *i*-Pr, CH2Ph; R2=CH3, Ph, Ind-3

Using the alkaloid Ajmaline **(9)** (from *Rauwolfia spp*. [10]), a known antiarrythmic and anti-inflammatory agent [11], we were able to obtain a homologous system **10** (yield for R=CH3 - 32%):



9 Ajmaline **10**

Analogs of the alkaloid Dregamine **(**from *Ervatamia spp*. [12]) can be obtained from the alkaloid Coronaridine D **11** (from *Tabernaemontana divaricata* [13]) by the alkylation of the latter with chloroketones and subsequent recyclization into compounds **12** (~35% at R=CH3 and 26% at R=Ph):



Coronaridine D (11) **12**

To sum up, the discovered recyclizations of semiaminals and related compounds represent novel methods for the formation of 3-benzazepine systems [14,15] and homologs, which allow direct synthesis of mimetics and structural analogs of hard-accessible alkaloids containing the azepine cycle.

The study was carried out using natural compounds from the collection of **InterBioScreen Ltd**. (www.ibscreen.com).

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O-19

Organocatalytic Asymmetric Synthesis of 1,2,4-Trisubstituted Azetidines By Reductive Cyclization of Aza-Michael Adducts of Enones

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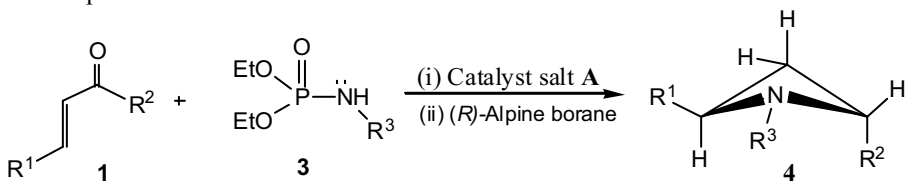
Over the years, functionalized aza-heterocycles, which are at the heart of many essential pharmaceuticals and physiologically active natural products, have attracted the attention of organic chemists in order to develop novel, synthetically useful, and elegant methodologies for the synthesis of such type of compounds as targets for design of new drugs and important intermediates in organic synthesis. Amongst chiral nitrogen heterocycles, azetidines [1,2] have received much attention during the last decade because of their utilization as ligands[3] and their biological and pharmaceutical activities.[4,5] Recently, G. Bartoli and P. Melchiorre have developed primary amine salt catalyst **A**[6] for both iminium ion catalysis and asymmetric counteranion-directed catalysis (ACDC) phenomenon,for the highly enantioselective conjugate addition of a series of different nucleophiles[7] (-C, -S, -O centered nucleophiles) to enones.[8] In our endeavors to synthesize enantiopure azetidines, we advanced this organocatalytic activation strategy to document an operationally trivial procedure for the aza-michael addition of of *N*-arylphosphoramidates **1** to a,ß-unsaturated ketones **2** catalyzed by the chiral salt **A** to give aza-Michael adducts **3** followed by the intramolecular reductive cyclization via (*R*)-Alpine borane to give 1,2,4-trisubstituted azetidines **4** (in 67-93% yield with 85-95% diasteroselectivity and 78-96% enantioselectivity) in a one-pot procedure as outlined in Scheme 1. To the best of our knowledge, primary amine salt **A** has not been used for the conjugate addition of nitrogen nucleophiles to enones till date and

herein we report the first organocatalytic addition of phosphoramidates (a weak nitrogen containing nucleophile) to enones ultimately leading to enantiopure azetidines **4**.



Scheme 1 synthesis of enantiopure trisubstituted azetidines

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O-20

Regioselective Synthesis of Pyrrolo[1,2-*a*]quinolines via Electrophilic Cyclization/[3 + 2] Annulation with Concomitant Ring Opening of Iodo-Pyranoquinolines

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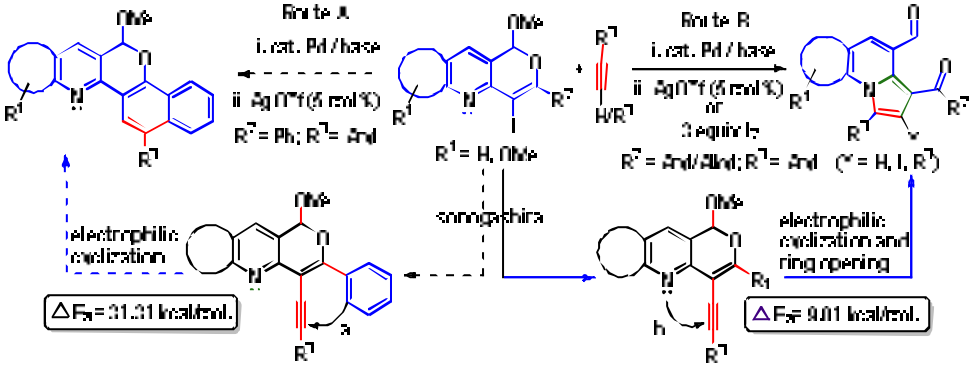
We have designed a novel strategy for the synthesis of highly functionalized pyrrolo[1,2-*a*]quinolines and indolizines from pyranoquinolines [1] via site-selective electrophilic cyclization and subsequent ring opening of pyran ring using transition metal/ iodine under mild reaction conditions.[2] Halogenated heterocyclic compounds serve as a useful platform for increasing the molecular diversity. In this context, we have introduced iodide functionality in the molecule by the electrophilic iodocyclization. This approach involves the preferential attack of pyridyl nitrogen over aryl ring and leads to the formation of 5-*endo*-*dig* cyclized products. Our results are supported by quantum chemical calculations between C-N and C-C bond of the substrate and further by the X-ray crystallographic analysis. Developed chemistry also leads to the formation of [3+2] alkyne annulated products[3] while, the reported electrophilic cyclization involves [4+2] annulation through the CH activation of adjacent aromatic carbon.[4] In the alkyne annulations, the symmetrical and unsymmetrical internal alkynes afforded the single isomers selectively. As the nitrogen-containing heterocycles and their analogues are pharmaceutically important scaffolds.[5] This methodology provides facile access to a range of pyrrolo[1,2-*a*]quinolines and indolizines which should be useful in medicinal chemistry and diversity oriented synthesis. The reported indolizine derivatives are associated with a wide range of biological activities including anticancer, antibacterial, antifungal, anti- tubercular and anti-histaminic, cytotoxic and CNS depressant activity.[6]



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O-21

SYNTHESIS OF HETERO RING CONDENSED SOME CARBAZOLES & AZACARBAZOLES

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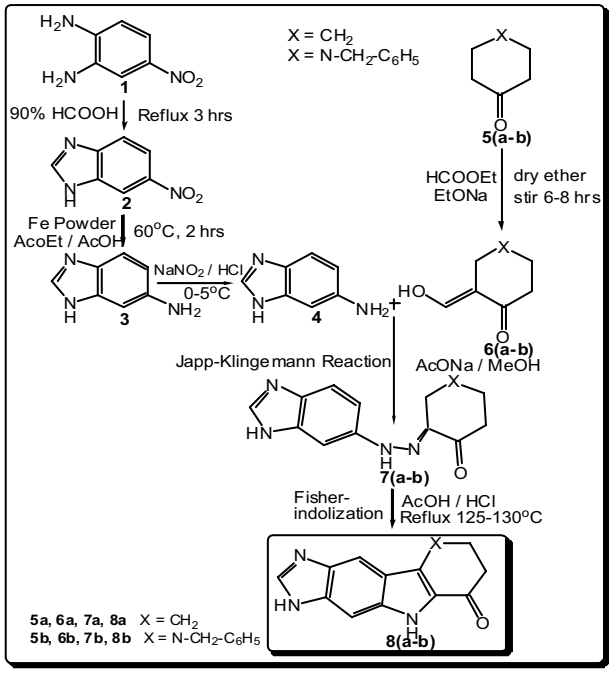
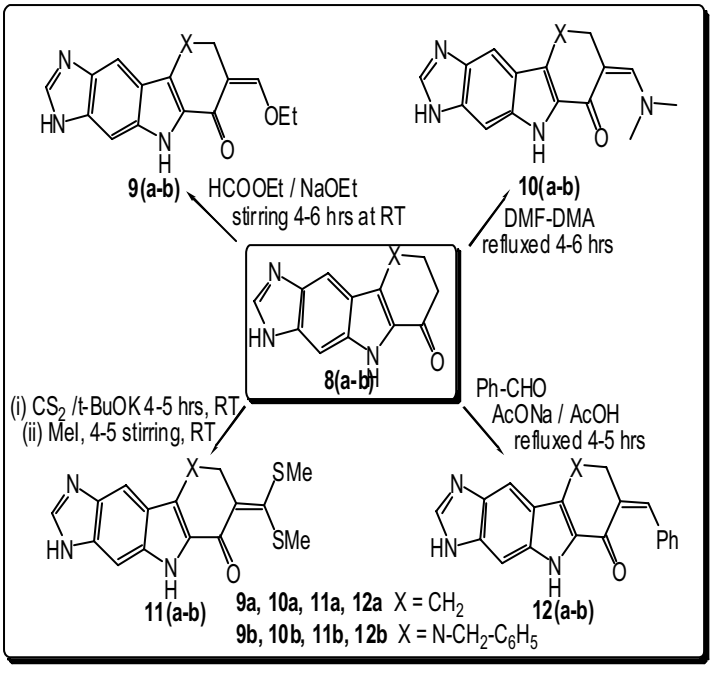
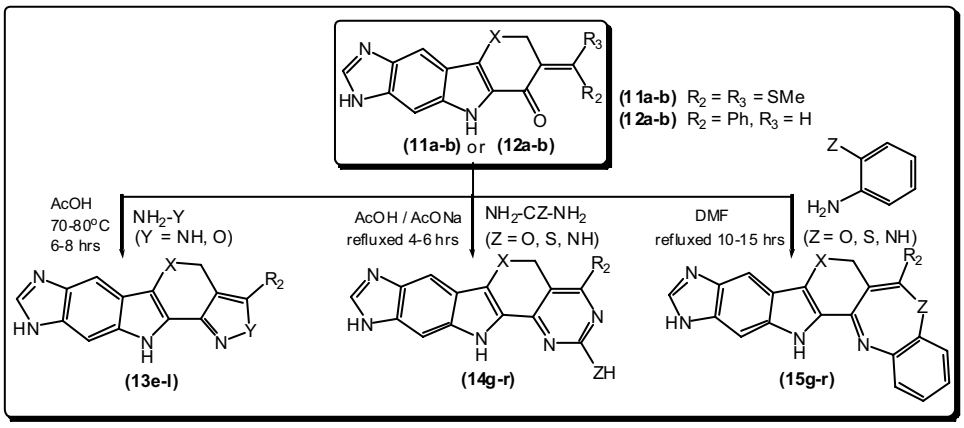
Application of Japp-Klingemann reaction with benzimidazolyl diazonium chloride **(4)** on 2-hydroxymethylidene cyclohexanone **(6a)** and *N*-benzyl-3-hydroxymethylidene-4-piperidone **(6b)** yielded the corresponding hydrazones **(7a-b)** which underwent facile Fischer-indolization in acid to give the imidazo condensed oxocarbazole and imidazo condensed oxoazacarbazoles **(8a-b).** Subsequent treatment of **(8a-b)** with (i) HCOOEt, NaOEt (ii) C6H5CHO (iii) CS2, CH3I, NaOEt and (iv) $Me_2NCH(OMe)_2$ yielded in succession the corresponding enolic ethers **(9a-b)**, dimethylaminomethylene ketones **(10a-b)**, oxoketenedithioacetals **(11a-b)** and a,ß-unsaturated ketones **(12a-b)** respectively. Interaction of **(9a-b), (10a-b), (11a-b)** and **(12a-b)** with bidentate nucleophiles such as hydroxylamine hydrochloride and hydrazine hydrate afforded the corresponding isoxazolo and pyrazolo incorporated derivatives of imidazo condensed carbazoles and azacarbazoles **(13a-l).** Similar interaction with urea and thiourea yielded corresponding pyrimido incorporated imidazo condensed carbazoles and azacarbazoles **(14a-r).** Reactions of these intermediates with *o*-phenylenediamine, *o*-aminophenol and *o*-aminothiophenol produced benzodiazepino, benzoxazepino and benzothiazepino incorporated imidazo condensed carbazoles and azacarbazoles **(15a-r)** respectively. Structures of all the compounds have been unequivocally established on the basis of their elemental and spectral data. Antifungal and antibacterial activities of some of the synthesized compounds have been carried out.






(11a-b) or (12a-b)
(11a-b) R2 = R3 = SMe
(12a-b) R2 = Ph, R3 = H
AcOH
70-80°C
6-8 hrs
NH2-Y
(Y = NH, O)
AcOH / AcONa
refluxed 4-6 hrs
NH2-CZ-NH2
(Z = O, S, NH)
DMF
refluxed 10-15 hrs
(Z = O, S, NH)
(13e-l)
(14g-r)
(15g-r)

❑❑❑

Abstracts of Poster Session

PP-101

Determination of Iron with 3-hydoxy-3-methyl-1-p-methoxy phenyl triazene

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ABSTRACT

3-Hydoxy -3-methyl-1-p-methoxy phenyl triazene has been prepared[1] (m.p. 102^0C) by coupling methyl hydroxylamine with diazonium salt in 1:1 molar proportion at 0-5^0C. The reagent solution was prepared in ethanol. The standard solution of iron was prepared by dissolving requisite quantity of A.R. grade ferric nitrate nona hydrate in double distilled water. To prevent hydrolysis a few drop of concentrated nitric acid were added to the solution. The solution was then standardized with EDTA using sulphosalicylic acid as an indicator[2]. A systronics UV-VIS spectrophotometer-108 was used for spectrophotomrtric work and for pH-measurements systronics pH meter-324 was used.

The green Fe(III) complex was soluble in ethanol and its color was stable for more than 24 h. It gives maximum absorbance at 730 nm therefore subsequent absorbance were made at 730 nm against solvent blank. Six fold excess of the reagent was used and pH was kept between 2.0 to 3.0. The system obeys Beer's law in the range from13.96 ppm to 27.92 ppm of iron. Sandell's sensitivity is 43.93 ng/cm^2 and molar absorptivity is 1,270 liter/mole cm. The Job's method[3], Slope ratio method[4] and mole ratio methods- (i) Yoe & Jones[5] and (ii) Zolotov's[6] gave 1:3 (Fe:R) stoichiometery for the complex. Interference of 26 diverse ions was studied in determination of 13.90 ppm of iron. Na(I), K(I), Ba(II), NH_4^+, Cl^-, Br^- and SO_4^- did not interfere when present in 100 ppm concentration. In addition to these ions, Mn(II), Ni(II), Cd(II), I^- and CO_3^{--} did not interfere when present in -10 ppm. The precision study was carried for 13.96 ppm of Fe(III), standard deviation was 0.096 ppm of iron. The solid complex was obtained as blue micro crystal, m.p. 147^0C with molecular formula $Fe(C_8H_{10}N_3O_2)_3$. This molecular formula corroborates the composition of the complex found with solution studies.

PP-102

Corrosion Inhibition of Tin in 1N HCL By *Tribulus terrestris* seed Extract

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ABSTRACT

The inhibition of corrosion of Tin metal using Gokhru (Tribulus terrestris) extract in 1N HCl solutions was studied by mass loss method at ±30°C. The result showed that corrosion rate was significantly decreased in presence of the methanolic extract of plant part (i.e. seed) and inhibition efficiency increased with increasing the concentration of plant extract. Corrosion inhibition could be explained by considering an interaction between metal surface and the inhibitor molecules. The inhibition action of T. terrestris (Tt) extracts is due to their adsorption on the metal surface.

PP-103

Gold nanocrystals Stabilized on Montmorillonite clay: An efficient Heterogeneous Catalyst for the one-pot synthesis of Propargylamines

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ABSTRACT

In the recent years, there has been increasing interest in 'gold' for use as catalysts in organic transformations, though gold was traditionally considered to be chemically inert and regarded as a poor catalyst. The development of nanometer sized gold nanoparticles is intensively pursued because of their importance for both fundamental science and advanced technology. The performance of nanoparticles in different aspects is dependent on the size, shape and the supporting materials on which these nanoparticles are stabilized. In the present work, we have reported *in situ* generation of crystalline Au^{o}-nanoparticles into the nanopores of acid activated Montmorillonite clay and their catalytic performance in one-pot, three component (A^3) condensation of an Aldehyde, an Amine and an Alkyne *via* C-H alkyne-activation to synthesize propargylamines [Scheme 1]. Propargylamines are versatile intermediates for the preparation of various nitrogen-containing compounds and are important components of biologically active pharmaceuticals and natural products. The activation of Montmorillonite clay was carried out with HCl under controlled conditions for generating nanopores into the matrix and these nanopores act as "host" for *in situ* generation of Au^{o}-nanoparticles. The synthesis consisted of impregnation of the acid-activated Montmorillonite clay with $[AuCl_4]^-$ solution and reduction with $NaBH_4$. The synthesised Au^{o}-nanoparticles crystallized in the face centred cubic (fcc) lattice were single crystals with a preferential growth direction along the (111) plane. The Au^{o}-nanoparticles serve as efficient *green* and heterogeneous catalyst for one-pot synthesis of propargylamines with excellent yields and selectivity under mild reaction conditions.

PP-104

COMPARATIVE THERMOACOUSTIC STUDY OF SOLUTIONS OF AMINO ACID L-THREONINE WITH UREA(aq) AND WITH UREA(aq)+KBr(aq)

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ABSTRACT

Acoustic performance is an important method to determine the intermolecular interactions. Amino Acids that must be obtained from the diet are called "Essential Amino Acids" other Amino Acids that the body can manufacture from other sources are called "Non Essential Amino Acids." L-Threonine helps maintain proper protein balance in the body. Urea serves an important role in the metabolism of nitrogen-containing compounds by animals and is the main nitrogen-containing substance in the urine of mammals. Potassium Bromide is used as an antiepileptic medication as explained by Mehraet al.

The variation of density, viscosity and sound speed data with amino acid L-Threonine taken as solute has been studied with respect to various thermoacoustic, volumetric and viscometric properties by experimental procedures using precalibrated bicapillary pyknometer, precalibrated Ostwald's viscometer and precalibrated Ultrasonic interferometer respectively. The error values are ±0.06% for density measurements, ±0.07% for viscosity measurements and ±0.04% for sound speed as reported throughout the experimental work. The data is further utilized to calculate parameters viz. adiabatic compressibility (ß), apparent molar volume (F_v), apparent molar compressibility (F_k), acoustic impedance (Z), intermolecular free length (L_f), Relative Association (R_a). The concentration selected for amino acid is upto maximum solubility of solute. The values for viscosity coefficient A and B of Jones-Dole equation, Masson's equation are also derived. The measurements are conducted at three temperatures viz. 298, 308, 318K. The results are studied on the basis of solute-solvent interaction and study is based on graphs, which clearly reveals the structure associative or dissociative nature of the solute-solventas discussed by Mehra et al.

PP-105

FREE RADICAL SYNTHESIS OF HALOGEN CONTAINING POLY MALEIMIDES AND ITS THERMAL AND ANTIMICROBIAL STUDIES

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ABSTRACT

The copolymer (C-CFPMI1) of 3-Chloro 4-flouro (phenyl) maleimide (N-CFPMI) and copolymer (C-CNPMI1) of 2-Chloro 4-nitro (phenyl) maleimide (N-CNPMI) with methylmethacrylate a was prepared free radically at 70°C using Dimethylfuran (DMF) as a solvent and Benzoyl peroxide (BPO) as free radical initiator. The copolymers composition was determined by N - elemental analysis. Effect of solvent, free radical initiator, time on polymers yield was also studied. Both the polymers are characterized by FT -IR and ^{1}H NMR data. The intrinsic viscosity of C-CFPMI1 and C-CNPMI1 in DMF solution was 0.2140dL/g and 0.0873dL/g. Thermogravimetric analysis (TGA) characterizes the thermal stability of copolymers. Activation energy were calculated using freeman Caroll method.The order of copolymerization was of first order. The initial decomposition temperature (T_i) for C-CFPMI1 and C-CNPMI1 was 160^{o}C and 150 ^{o}C.The activation energy for C-CFPMI1 and C-CNPMI1 are The gel permeation chromatography (GPC) determines the molecular weight and polydispersity index (PDI) of the two polymers. Molecular weight observed for C-CFPMI1 and C-CNPMI1 was 3619.3 and 2616 and polydispersity index (PDI) was1.4872 and 1.372. The antimicrobial activities of copolymers were also investigated against various microorganisms.

PP-106

13-hydroxy-ß-amyr-20-ene from fruit of *Osbeckia chinensis*

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ABSTRACT

Due to both climatic and geographical variation the Sub-Himalayan region of North East India is endowed with vast flora & fauna. *Osbeckia chinensis* (Melastomaceae), a widely distributed species of this region reported have several medicinal uses. Some, compounds have already been isolated from this plant. The plant has also a good traditional importance among the people of North-east India. As a part of our ongoing studies on bioactive secondary metabolites from the flora of this region.we have investigated *O. chinensis* and isolated 13-hydroxy-ß-amyr-20-ene along with ß-sitosterol , rutin from the fruit of the plant. Antifungal potential of the compounds were also measured against *Alternaria alternata*. Minimum Inhibitory Concentration (MIC) for 13-hydroxy-ß-amyr-20-ene, ß-sitosterol and rutin were also determined. The details of work done on this plant will be presented.

PP-107

Long Straight Chain Compounds from Flora of North East India

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ABSTRACT

In continuation of the ongoing programme of CSIR-NEIST, Jorhat in search of bioactive molecules from Sub-Himalayan region of North East India, 3 medicinal plants, namely, *Cinnamomum obtusifolium, Elaeocarpus lanceifolius and Baccaurea sapida* were investigated. This study yielded several very long chain alkane derivatives. The structures of the isolated compounds were elucidated by spectroscopic methods. Compounds were also tested against two plant pathogenic fungi, *Alternaria tenuissima* and *Alternaria alternate*. The details of this investigation will be presented in this presentation.

PP-108

Antioxidant and antimicrobial effect of Ayurvedic formulation for management of diabetes

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ABSTRACT

Ayurvedic poly-herbal formulations are implemented in as a cost effective remedy for diabetes. The pharmacological principles in the formulation work together in dynamic way to produce maximum therapeutic efficacy with minimum side effects. The present study aimed to evaluate multi purpose formulation for the management of hyperglycemia and infections in diabetes. Aqueous and ethanolic extracts of poly-herbal formulations [1] were subjected to phytochemical screening. The quantitative analysis of phenolics and flavonoids was carried out. The free radical scavenging and antioxidant activity of the extracts was determined by DPPH free radical scavenging assay and FRAP assay respectively. The antimicrobial potential was evaluated by agar well diffusion method against Gram positive and Gram negative microorganisms.

The high amount of phenolics and flavonoids present in the poly-herbal extract suggest their antioxidant potential. A significant antimicrobial activity was obtained for aqueous extract suggesting the presence of a wide range of antimicrobial components. Therefore this Ayurvedic poly-herbal combination could be a complementary mode of management of hyperglycemia and infections in diabetic patients.

PP-109

Design, Synthesis and Evaluation of Cyanoguanidine based New Chemical Entities as IGF1R Inhibitors

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ABSTRACT

Insulin-like growth factor-1 receptor (IGF1R) is a member of the insulin receptor family of tyrosine kinases. Off late several small molecule inhibitors targeting IGF1R have entered various steps of clinical trial. Preclinical pharmacology supports IGF1R targeting as a viable anticancer therapy for various types of oncology indications. As part of a program to discover a novel chemical moiety for IGF1R inhibitors, we identified an open chain cynoguanidine core structure as IGF1R inhibitor. The cynoguanidine functionality is generally used as a bioisostere of urea and thiourea moieties. The cyanoguanidine moieties can be found in several biologically active agents such as Histamine - H2 antagonist and antihypertensive potassium channel activators etc. Furthermore, pyridylguanidine have been implicated for their antitumor activity[2]. In this poster we will describe the synthesis and preliminary SAR for a series of cyanoguanidine based new chemical entities.

PP-110

Synthesis of Novel Isocytosine Based Xanthine Oxidase inhibitors

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ABSTRACT

Gout is a disorder caused by deposition of urate crystals in joints and other tissues, and preceded by hyperuricemia. The commonly used xanthine oxidase inhibitors (XOIs), allopurinol and febuxostat are associated with an adverse effect that includes gastrointestinal, hepatic, renal and hematological toxicities, skin problems and allergic reactions.[1,2] Pegloticase, which

mops up the excess uric acid has recently been approved by US FDA for advanced cases of treatment-resistant gout is also having problem related to infusion reactions, cardiovascular events, allergic reactions and immunogenicity. Hence the search for better drugs, having fewer adverse effects, continues. Our work is focused on finding a novel class of XOIs which may avoid some of the adverse effects of drugs currently in the market.

Using virtual screening of in-house synthetic library followed by *in vitro* and *in vivo* testing led to the identification of a novel isocytosine scaffold for xanthine oxidase inhibitor, [4] which has features common to both allopurinol as well as febuxostat. We made various chemical modifications of the initial hit (IC_{50} 12.42 ± 0.5 µM) to improve the activity and PK profile using structure-based drug design (SBDD). Structure-activity relationship (SAR) studies were carried out on isocytosine scaffold for xanthine oxidase inhibitory activity and showed 470-fold improvement in *in vitro* IC_{50} compare to initial hit obtained in the process. Five most potent compounds with nanomolar *in vitro* IC_{50} values were taken forward for pharmacokinetic (PK) and in vivo experiments. *In vivo* results suggested requirement for improvement in PK properties of this series of compounds as the in vivo efficacy did not match expectations based on *in vitro* results. Chemical modifications aimed towards overcoming these liabilities will be presented.

PP-111

Synthesis of cyclobutan-1-one derivatives by the reaction of ketenes with chalcones

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ABSTRACT:

The reaction of haloketene and phenylketene with various chalcones and the chemistry of some of the reaction products have been investigated. The formation of cyclobutanone was taken as an indication that the reaction proceeds by an[2+2] cycloaddition in concerted mechanism. These all reactions create new opportunities to utilize the unique structures and high reactivity of ketenes for even greater progress in the future.

Organic compounds containing four member ring present a unique group of metabolites, including natural products and drugs. The cyclobutanone unit is found as a basic structure element in a wide range of naturally occurring compounds in bacteria, fungi, plants and marine invertebrates. Many biological activities are shown and may serve as potential drug leads or provide new idea for the study of enzyme mechanism and organic synthesis. Some cyclobutanone compounds such amino-acids, peptides, and nucleosides show protective properties against ultraviolet radiation. In the skin, many molecules may absorb UV radiation upon exposure.

Bacterial resistance to antibiotics is an emerging epidemic throughout the world and there is a need desperate need for new antibiotics and new strategies to maintain the effectiveness of current agents. Cyclobutanone analogues of ß- Lactam antibiotics were explored in the early 1980 as potential inhibitors of ß-Lactamases and D-Ala-D-Ala transpeptidases. Cyclobutanones have the potential to exhibit broad-spectrum inhibition of both serine and metallo-ß-Lactamases through the formation of enzyme bound hemiketals or hydrates.

Ionizing radiation e.g. ?-irradiation, for the preservation of foods is not generally accepted and allowed. The development of tests for the detection of irradiated foods is of importance in this matter.[12] Together with a good management at the irradiation facility, such tests would facilitate international trade and increase consumer confidance in the existing control procedures .The detection of 2-substituted cyclobutanones as markers for ?-irradiated foods proved to be very successful for chicken, peanuts, papaya, liquid whole eggpork, lamb, beefand fish.

From the above review, it can be said that cyclobutanone and their derivatives display a wide range of pharmalogical activities, such as antibacterial, anti-inflammatory and broad spectrum inhibition of both serine and metallo-ß-Lacamases with good protective properties against ultraviolet radiation. Because of this, chalcones and their derivatives have attracted increasing attention of the scientists for the search of new potent pharmalogical activity in it.

Keywords: Ketenes, chalcone, cycloadddition, concerted mechanism

PP-112

Design and Synthesis of Novel Anthracene based Molecules for Application in Organic light Emitting Devices

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ABSTRACT

Various substituted Anthracene based molecules were synthesized from Anthracene for application in organic light emitting devices. The salient features of this method include mild reaction conditions, high yields and large scale synthesis. Organic Light Emitting Devices (OLED) find vivid, versatile applications in the miniaturized electrical and electronic gadgets of modern era along with diverse biological attributes. The salient features of OLED demark them as better candidates over Light Emitting Diode (LED) and Liquid Crystal Display (LCD) systems. The products thus obtained have been characterized by mp, IR, ^{1}H NMR, and mass spectroscopy. The physical interpretation of OLED materials enable us to realize their potential applications.

PP-113

Designed synergy of chirality, charge and hydration modules: Synthesis of 2'-*O*-[*R*/*S*-(2-amino-3-methoxy)propyl] (*R*-AMP and *S*-AMP nucleic acids)

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ABSTRACT

The 2'-O-methoxyethyl substituted antisense oligonucleotides (MOE-AONs) are currently being studied [1] in several ongoing clinical trials and have shown excellent safety profiles. The success of MOE-AONs was attributed to the gauche interactions of vicinal 2'-*O*- and the methoxy- substitution, and protecting against hydrolytic cleavage due to steric hindrance in the minor groove. [2] The 2'-*R*-/*S*-AMP tethered AONs were efficiently achieved from L-serine and 2,2'-anhydrouridine. We chose a DNA sequence of biological relevance that was used in the splice-correction assay developed by Kole *et al*. [3] UV-T_m studies and SVPD digestion of these AONs were performed. The MOE-AONs are almost completely digested by SVPD at the end of 1h, whereas 90% of *R*-AMP-AON and 80% of *S*-AMP-AON are still intact and are effectively able to resist hydrolytic cleavage without compromising the DNA:RNA duplex stability. At the end of AONs digestion for 4h with SVPD, it was interesting to see that our designed amine chirality is also a contributing factor in protecting the AONs against SVPD.

The synergistic contributions of MOE together with the amino substituents and chirality effects towards RNA:DNA duplex stability and enzyme digestion are shown for the first time. We have thus transformed MOE modification into a synergy of chirality, positive charge and hydration module, all in one, in our design of *R*-/*S*-AMP AONs. The amino pendant groups have additional advantages also in improved kinetics of binding and efficient cellular uptake.[4] Further attention is warranted for this interesting analog, for applications in antisense as well as recently discovered single stranded siRNA technologies.

PP-114

SYNTHESIS OF 2-AMINOTHIAZOLES: ACTIVE SYNTHONS FOR MEDICINAL POTENT HETEROCYCLES

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ABSTRACT

The 2-aminothiazoles are useful intermediates in organic synthesis and active pharmacophores in the field of medicinal chemistry. Thiocynates derivatives of a-bromo keto compounds are useful intermediates in the synthesis of heterocyclic compounds such as thiazoles, oxazoles and pyrrols. Substituted a-bromoketo compounds were treated with potassium thiocynate in microwave condition to form phenacyl thiocynates. **(2a-d).** The phenacyl thiocynates **(2a-d)** were reacted with ammonium acetate to synthesize substituted 2-aminothiazoles **(3a-d)**. These 2-aminothiazoles will be used to synthesize substituted urea and subsequently 4-thiazolidinones. All the compounds have been characterized by IR, ^{1}H NMR and MS spectral data. The evaluation of biological properties of the compounds is in progress.

PP-115

Third-Party Observation: The Valuable Tool to Challenge the Legal Validity of Patent applications"

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ABSTRACT

Due to recent changes in the Intellectual Property laws worldwide, **third-party observations** is a valuable tool. Well-crafted observations can be highly valuable weapons in the battle of patent infringement issues. So the involvement of the public (as a third party) in patent examination is used in some forms to help identifying relevant prior art and, more generally, to help assessing whether patent applications and inventions meet the requirements of patent law, such as novelty, inventive step or non-obviousness, and sufficiency of disclosure. In some circumstances, they can also be readily coordinated with the respective patent office if required. Third party observations may be filed – without incurring official fees – by any third party with regard to a pending patent application or during an ongoing opposition against a granted patent. The submission of these observations provide the possibility that third parties directly point the prior art (patents, patent applications, or documents which are relevant to a pending patent application) once the patent applications are published, therefore these observations impacts the applicant, International Search/Examination Authorities, and Designated Offices during the pregrant and post grant examination. Compared to oppositions, **third-party observations** have been used, according to the informal evidence available. This might be due to concern that the observation filer is not a party to the proceedings and may have less influence than an opponent, or to concern that, if the examining division does not recognize the merits of an observation, making the same arguments later in an opposition may be more difficult. Oppositions, however, also have their own disadvantages. First, of course, the challenger must wait until a patent issues before acting. Second, oppositions can take years to resolve and can be relatively expensive to pursue, particularly if the matter is appealed. The result might be years of uncertainty, especially where the issued patent blocks freedom to operate in a critical area. On the other hand, a persuasive observation may clear a freedom-to-operate hurdle before any patent even issues, and at a much lower cost. Moreover, many companies now regularly track the prosecution of competitors pending patent applications on-line using the respective patent office website.

PP-116

SYNTHESIS OF FIVE-, SIX- AND SEVEN-MEMBERED HETERO RING ANNULATED IMIDAZO[4,5-B]CARBAZOLES AND AZACARBAZOLES

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ABSTRACT

Application of Japp-Klingemann reaction with benzimidazolyl diazonium chloride **(4)** on (i) 2-hydroxymethylidene cyclohexanone **(6a),** (ii) 3-hydroxymethylidene-4-piperidone **(6b)** and (iii) N-benzyl-3-hydroxymethylidene-4-piperidone **(6c)** yielded the corresponding hydrazones **(7a-c)** which underwent facile Fischer indolization in acid to give the imidazo condensed oxocarbazole **(8a)** and imidazo condensed oxoazacarbazoles **(8b-c).** Subsequent treatment of **(8a-c)** with (i) HCOOEt, NaOEt (ii) C_6H_5CHO (iii) CS_2, CH_3I, NaOEt and (iv) $Me_2NCH(OMe)_2$ yielded in succession the corresponding enolic ethers **(9a-c)**[3], α,β-unsaturated ketones **(10a-c)** [4], oxoketenedithioacetals **(11a-c)** and dimethylaminomethylene ketones **(12a-c)**[6] respectively. Interaction of **(9a-c), (10a-c), (11a-c)** and **(12a-c)** with bidentate nucleophiles such as hydroxylamine hydrochloride and hydrazine hydrate afforded the corresponding isoxazolo and pyrazolo incorporated derivatives of imidazo condensed carbazoles **(13a-c)** and azacarbazoles **(13d-f).** Similar interaction with urea and thiourea yielded corresponding pyrimido incorporated imidazo condensed carbazoles **(14a-b)** and azacarbazoles **(14c-f).** Reactions of these intermediates with *o*-phenylenediamine, *o*-aminophenol and *o*-aminothiophenol produced benzodiazepino, benzoxazepino and benzothiazepino incorporated imidazo condensed carbazoles **(15a-c)** and azacarbazoles **(15d-i)** respectively. Structures of all the compounds have been unequivocally established on the basis of elemental and spectral data. Biological screening of the compounds is in progress.

PP-117

Synthesis and Antiplatelet Activity of Bicyclic Diamine Derivatives of N-Substituted Pyroglutamic Acids

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ABSTRACT

Thrombotic disorders are the major cause of morbidity and mortality in the developed world, while their incidents are rapidly taking the upper hand in developing countries. Platelets have a crucial role in haemostasis and thrombosis. By understanding the multifaceted mechanisms involved in platelet interactions with vascular surfaces and aggregation, new approaches can be tailored to selectively inhibit the pathways most relevant to the pathological aspects of atherothrombosis.The structural features of conformationally restricted diamines (CRDA) have already proved their advantages in drug design. The present study furnishes cyclic diamine derivatives of substituted *S*-pyroglutamic acid moieties as inhibitors of collagen induced platelet adhesion and aggregation mediated through collagen receptors. Therefore, carboxamide derivative of confirmationally rigid, substituted bispidine with different N-araalkyl pyroglutamic acids were prepared as target compounds and their collagen induced antiplatelet aggregation activity were screened both *in vivo* and *in vitro*. 14 pyroglutamides showed 40-60 % protection at 30µm concentration, while the standard antithrombotic drug Aspirin displayed only 40% protection at the same dose, by collagen plus epinephrine induced pulmonary thromboembolism in mice (*in vivo*). Seven compounds showed highly promising anti-platelet efficacy inhibited by collagen (*in vitro*). Comprehensive study suggests that these compounds display remarkable antithrombotic efficacy much better than the existing anti-platelet drugs, with a moderate alteration in bleeding tendency.

PP-118

New metal–based cancer chemotherapeutic glycoconjugate derived from N–glycoside scaffold: DNA binding profile, topoisomerases activity and in vitro cytotoxic activity against different human cancer cell lines

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ABSTRACT

To explore the prospect in cancer therapy of metal based drug, new carbohydrate–conjugate heterobimetallic complexes $[C_{32}H_{62}N_{10}O_8NiSn_2Cl_4]$ (**3**) and $[C_{32}H_{62}N_{10}O_8CuSn_2Cl_4]$ (**4**) were synthesized from their monometallic analogs $[C_6H_{16}N_4O_2CuCl_2]$ (**1**) and $[C_6H_{16}N_4O_2NiCl_2]$ (**2**) containing N,N′–di–ß–D–glucopyranosyl ethylenediamine N-glycoside ligand (**L**) and were characterized by various spectroscopic and analytical methods. The *in vitro* DNA binding studies of ligandandcomplexes (**1**–**4**) with CT–DNA were carried out by employing various biophysical and molecular docking techniques which revealed that complexes **3** and **4** strongly bind to DNA in comparison to monometallic the free ligand. Cleavage studies employing gel electrophoresis demonstrate that both the complexes **3** and **4** are specific groove binders and cleave supercoiled pBR322 DNA via hydrolytic pathway, which was further confirmed by T4 DNA ligase assay. Complex **3** inhibited Topo–II mediated relaxation activity in a dose–dependent manner that appeared in accordance with remarkably good anti–tumor activity against MIAPACA2, A498 and HCT15 tumor cell lines (GI_{50} < 10mg/ml) and therefore, emerged as an important antineoplastic and antiproliferative agent. Finally, complex **3** wasdocked into the ATPase domain of human–Topo–II in order to probe the possible mechanism of inhibition.

PP-119
MODIFIED CLAY SUPPORTED Ni^{O}-NANOPARTICLES: AN EFFICIENT AND REUSABLE CATALYST FOR SELECTIVE REDUCTION OF CHLORONITROBENZENE

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ABSTRACT
Metal nanoparticles have attracted great attention in recent time for their unique size dependent properties and applications in the fields of catalysis, coatings, magnetic devices, drug delivery etc. [1-3]. Due to stringent and growing environmental regulations, chemical industry needs the development of ecofriendly synthetic methods. The development of environmentally sustainable synthetic methods and the choice of suitable support towards the synthesis of metal nanoparticles having uniform size distribution with different shapes and exposed facets are key importance for the exploration of new research. We report here the *in situ* generation of Ni^{o}-nanoparticles into the nanopores of modified Montmorillonite clay matrix by hydrazine reduction of impregnated $NiCl_2$-clay composite in ethyleneglycol at 60°C [4]. The modification of Montmorillonite clay was carried out by activating with H_2SO_4 under control conditions to achieve desired pore size and high surface area [5]. The acid activated Montmorillonite showed micro- and mesopores with the pore diameters in the range of 0-8 nm, a high specific surface area up to 679.1 m^2/g and specific pore volume 0.69 cm^3/g. The morphology of Ni^{o}-nanoparticles was studied by means of Powder XRD, TEM, SEM-EDX and Surface area measurements. XRD pattern of Ni^{o}-nanoparticles revealed the formation of face centered cubic (fcc) lattice. The Ni^{o}-nanoparticles supported on modified Montmorillonite are found to catalyse hydrogenation of ortho, meta and para chloronitrobenzene to corresponding chloroanilines with conversion 96.4, 99.7, 97.0 % respectively and selectivity nearly 100 % after 1 h reaction time (Scheme 1). The catalyst can be reused without significant loss of their activity.

PP-120
Preclinical pharmacokinetics and tissue distribution study of anti-tubercular azolyl phenyl cyclopropyl methane, S010-399, in rats

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ABSTRACT
Tuberculosis (TB) is more prevalent in the world today than at any other time in human history. India alone accounts for an estimated one fifth (21%) of all TB cases worldwide [1,2]. The compound S010-399, an azolyl phenyl cyclopropyl methane derivative, has shown anti-tubercular activity (MIC, 3.25 µM). Therefore, the pharmacokinetics and tissue uptake of of the compound was carried out in rats to develop it as a potential candidate drug.

Young and healthy male *Sprague Dawley* rats were administered a suspension formulation of the compound at 10 mg/kg oral dose. Blood, lung (target organ), liver (major metabolic site) and spleen (organ of regeneration) were collected up to 24 h post dose. A rapid, sensitive and simple HPLC assay method in rat serum, lung, liver and spleen was developed and validated as per US-FDA guidelines [3] with detection limit of 10 ng/ml and was applied for bioanalyses of S010-399.

S010-399 was found stable in SGF, SIF and rat serum. After per-oral dosing, its absorption was rapid with a peak concentration (179.9 ± 6.6 ng/ml) at 2 h and low clearance (0.003 L/h/kg; [4]). It was widely distributed to liver, lung and spleen with high mean residence time (MRT) in all four biological matrices from 8-9.6 h. S010-399 showed higher drug distribution in liver (16.62 fold), lung (4.10 fold) and spleen (2.26 fold) than serum demonstrating that it exhibits fast absorption, high volume of distribution without extra hepatic elimination and with favourable targeted tissue distribution properties. The details will be presented.

PP-121

A NEW ONE-POT ORGANOCATALYZED ROUTE TO STEREOSELECTIVE SYNTHESIS OF 2-HYDROXYAZETIDINES AND 2-HYDROXYPYRROLIDINES

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ABSTRACT

Nitrogen heterocycles are of immense importance not only as key components of a range of bioactive compounds, both naturally occurring and synthetic, but also as synthetic precursors to a variety of pharmaceutically and industrially relevant nitrogen-containing compounds. In particular, azetidines and pyrrolidines are ubiquitous in nature, and the search for new synthetic methodologies for their substituted and chiral ring systems would be of significant value. Substituted azetidines are unique heterocycles that have a wide range of synthetic applications, remarkable biological activities, and are prevalent in natural products. Similarly, the literature survey revealed that the hydroxy pyrrolidine ring system is present in many biologically active alkaloids. In continuation of our ongoing efforts to develop synthetically useful organocatalytic processes, including the synthesis of small ring heterocycles [1], a straightforward asymmetric synthesis of a new series of 2-hydroxyazetidines/2-hydroxypyrrolidines with promising results obtained in terms of yields and excellent diastereo- and enantioselectivity was developed via enamine catalysis using diphenylprolinol silyl ether. The aza-Henry reaction of chiral enamines with various aldimines/aziridines under mild conditions followed by intramolecular hemiaminalisation affords the desired products 2-hydroxyazetidines **5** and 2-hydroxypyrrolidines **6**, respectively, in a one-pot operation. It was gratifying to find that the formation of 2-azetidinols/2-pyrrolidinols was entirely diastereoselective in favour of 2,4-*cis*/2,5-*cis* isomers, respectively. Realizing the concept of organocatalyzed addition of enamines formed *in situ* to imines as acceptors, Hayashi et al.[2a,b] and others[2c,d] have already reported the formation of *β*-amino compounds. The scope and generality of the reaction was adequately investigated and the conditions were optimized extensively. The synthetic protocol presents the first chiral amine triggered synthesis of 2-azetidinols and 2-pyrrolidinols via an anionic domino process, thereby it also widens the scope of synthetic utility of organocatalysis.

PP-122

On-Line HPLC – CD investigations of *Cis*-Pterocarpans and their Osteogenic Activity

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ABSTRACT

Pterocarpans, a potent phytoalexin [1], i.e. a defensive substance produced by plants in response to biotic and abiotic elicitors, which are used for their antitoxin and antifungal activities [2]. Pterocarpans possess a wide range of activities such as antibacterial, [3] antifungal [2] and osteogenic activities [4,5]. At as low concentration as 10^{-10} M, Pterocarpan (Medicarpin) suppressed osteoclastogenesis in bone marrow cells (BMCs). Pterocarpans induced apoptosis of mature osteoclasts isolated from long bones [6]. Online HPLC-CD method in combination with modern high-level quantum chemical CD calculations are used as a tool for the stereochemical assignment of numerous natural and synthetic chiral compounds. The first successful enantiomeric resolution of racemic pterocarpans (medicarpin and related compounds) by chiral HPLC was described by Antus et al. [7] During their experiments using methanol on Chiralpack OT(+) columns, they observed that some polymeric impurities eluted with the compounds leading to disturbances in ECD and UV measurements. Therefore we developed an improved method for the resolution of the enantiomers, for racemic *Cis*-pterocarpans and investigated the absolute configuration through on-line HPLC-CD in combination with Quantum calculation and osteogenic activity of *rac*- Pterocarpan and their pure enantiomers [8].

PP-123

PHARMACOPHORE MODELING, VIRTUAL SCREENING, MOLECULAR DOCKING, 3D-QSAR, SYNTHESIS AND *IN-SILICO* ADMET STUDIES OF AURORA KINASE-A INHIBITORS AS POTENTIAL ANTICANCER AGENTS

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ABSTRACT

Aurora kinases are important regulators of mitosis and over expressed in human cancers. Their aberrant expression leads to chromosomal instability and derangement of multiple tumor suppressors [1]. In this research, pharmacophore modeling was performed on 6 diverse molecules using GASP module of Sybyl X1.2 [2]. Among 4 generated models, model-2 was considered as the best having highest score. A refined model contains 4 features viz. 1 H-bond donor, 1 H-bond acceptor, 1 aromatic and 1 hydrophobic region. This model was used as a query for virtual screening in NCI database. A total number of 47053 molecules were obtained after Lipinski filtering. From results, 30 molecules were designed by knowledge based structure activity relationship study and were docked on co-crystal structure of Aurora kinase A (PDB ID: 3D14) to predict the binding orientation of drug candidates to their protein target. From this, 5 different substituted mercapto-purine derivatives were synthesized and characterized by FTIR, ^{1}HNMR and Mass. Anti-cancer activity was carried out using various cell lines. 3D-QSAR studies (CoMFA and CoMSIA) were conducted on a series of 30 compounds [3]. The best prediction were obtained with a CoMFA (q^2 = 0.632, r^2 = 0.984) and with CoMSIA (q^2 = 0.546, r^2 = 0.982). Both models were validated by a test set of 5 compounds producing good predictive r^2 values of 0.674 and 0.572, respectively. *In-silico* ADMET studies were carried out using OSIRIS property explorer. The designed compounds showed good potential to be Aurora kinase A inhibitors.

PP-124

BIOINFORMATICS: “BLAST” REVIEW

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ABSTRACT

Basic Local Alignment Search Tool (BLAST) is the online database searching and alignment software most frequently used for comparing nucleotide and protein sequence similarity and calculate statistical significance between matches. The comparison of nucleotide or protein sequences from the same or different organisms is a very powerful tool in biology. By finding similarities between sequences, we can predict the function of newly sequenced genes, proteins and explore evolutionary relationships between them. Now that whole genomes are being sequenced for many organisms, sequence similarity searching can be used to predict the location and function of protein-coding and transcription-regulation regions in genomic DNA. BLAST is used by input a nucleotide or protein sequence as a query into the textbox on one of the BLAST web pages against all the public sequence databases. This sends the query over the Internet, the search is performed on the NCBI databases and servers, and the results are posted back to the person's browser in the chosen display format.My podium will focus on how BLAST works, its output, and how both the output and program itself can be manipulated and how to use BLAST or interpret BLAST results easily.

PP-125

Total Synthesis of a natural anti-malarial, Aplidiopsamine A

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ABSTRACT

Aria is an infectious disease caused by protozoa of the genus *Plasmodium* and transmitted by the *anopheles* mosquito. Among the five pathogenic species, *Plasmodium falciparum* is most lethal. Although this disease can be prevented and treated, it still kills more than one million people every year[1]. Increasing resistance to the existing drugs poses a major problem hence continuous effort is required for new and more effective antiplasmodial drugs. Recently several antiplasmodial compounds have been isolated from natural sources, containing rarely seen 3*H*-pyrrolo[2,3-*c*]quinoline scaffold. Among these isolated alkaloids are marinoquinolines[2], trigononine B[3] and aplidiopsamine A[4]. Aplidiopsamine A was isolated from the temperate Australian ascidian, *Aplidiopsis confluata*. It is the first alkaloid to possess the tricyclic aromatic substructure 3*H*-pyrrolo[2,3-*c*]quinoline attached through a methylene bridge to an adenine. This compound exhibits significant inhibition of growth of chloroquine resistant and sensitive strains (3D7, Dd2) of the malaria parasite *Plasmodium falciparam*, and minimal toxicity towards human cells. Synthesis was carried out in three steps by using *o*-nitrostyrene as the starting compound. In the first step synthesis of pyrrole ring was carried out by reaction with toluenesulfonylmethyl isocyanide (TosMIC). The reduction of nitro group, followed by Mannich reaction with adenine aldehyde constitutes the second and third step, respectively. Details of the research work will be provided in the poster.

PP-126

Formulation Development & Evaluation of Mucoadhesive buccal patch of Venlafexine Hydrochloride

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ABSTRACT

The Aim of present work was to formulate Mucoadhesive buccal patches of Venlafexine Hydrochloride .The buccal region of the oral cavity is an attractive target for administration of the drug of Choice for increase bioavailability and prevent first pass metabolism of drug. Venlafexine Hydrochloride patches were prepared using HPMC K15, HPMC K100, PVP K30 Carbopol934. Formulations were prepared using 2^3 Factorial Design by YATE's method. FTIR and DSC data revealed that there is no interaction between Venlafexine Hydrochloride and polymers. The patches were evaluated for their thickness, Uniformity content, folding endurance, weight uniformity, Swelling index, tensile strength and surface pH. In-vitro studies of Venlafexine Hydrochloride -loaded patches in phosphate buffer (pH 6.8) exhibited drug release in the range of 84 to 99% in 8 hrs. Data of In-vitro release from patches were fit in to different mathematical models to explain kinetics. The models used were zero and first-order equations, Higuchi and Korsmeyer-peppas models. The Ex-vivo release study showed that patches could deliver drug to the oral mucosa. The results indicate that the mucoadhesive buccal patches of Venlafexine Hydrochloride may be good choice to bypass the extensive hepatic first pass metabolism with an improvement in the bioavailability of Venlafexine Hydrochloride through buccal mucosa.

PP-127

A study of the pharmaceutical application of Guar gum in oral controlled release tablets for water-soluble drugs

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ABSTRACT

Guar gum, a non-ionic polysaccharide is used to develop oral-controlled release tablets for water- soluble drugs with constant release rate. Roth et al[1] reported that sustained drug delivery has an edge over conventional formulations as it reduces dosing frequency and side effects through reduced fluctuations in blood plasma levels of drug and a time tailored efficacy profile

which results from release characteristics of the active ingredient into the blood stream. In the present study, an attempt has been made to compare the viscosity of different grades of guar gum obtained from Sriganganagar (S-1), Bikaner (S-2) and Nagaur (S-3) districts of Rajasthan, India. The gum swells rapidly by dissolution and forms a viscous gel. Bonferoni et al [2] and Kurahashi et al [3] studied that viscosity plays an important part in controlling the release of drug. The viscosity of guar gum solutions is dependent on time and pH. In dilute solutions the viscosity increases linearly for concentrations up to 0.5%, but, mineral acids and strong alkaline solutions reduces the viscosity Guar gum obtained from Sriganganagar (S-1) proved to be more viscous at pH 6-7.Sriganganagar, forms the North-western plain of Rajasthan having suitable, fertile soil. The gradual degradation in the properties of guar was observed while descending towards east of Rajasthan
The pharmaceutical properties of guar gum lack due to fall in viscosity as per other parameters, but, these can be overcome by modifying and derivatization of guar gum. Derivatives of guar gum are more viscous with constant viscosity.

PP-128

Isatin derivatives substituted tetracyanoquinodimethanes as novel Optical molecular materials

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ABSTRACT

Isatin is an indole derivative and the Schiff base of isatin are investigated for their pharmaceutical properties. Isatin has a characteristic of a dye. We are exploring the optical and semiconducting properties of substituted TCNQ's, From this point of view, we have treated the nitro, methyl and chloro derivatives of isatin with TCNQ and this resulted in the di-substituted TCNQ compounds namely, **(A)** 2-(4-(bis(5-nitro-2,3-dioxoindolin-1-yl)methyl)phenyl)malononitrile, **(B)** 2-(4-(bis(5-methyl-2,3 dioxoindolin-1-yl)methyl)phenyl malononitile and **(C)** 2-(4-(bis(5-chloro-2,3-dioxoindolin-1-yl)methyl)phenyl) malononitrile. We have prepared the di-substituted TCNQ's with different synthetic strategy, rather than the usual direct addition of amine to the TCNQ in solution state. The isatin derivative, a secondary amine (0.177g, 0.979mmol) was dissolved in 7ml DMF. The temperature was then decreased and maintained between 0-5^{0}C, before the addition of the base. Diazabicyclo-1,6 undeca-7-ane (DBU) (147 mmol) was added into the amine and stirred till room temperature was attained. TCNQ (100mg, 0.484 mmol) was then added and the temperature was increased to 80-90^{0}C. The reaction mixture was stirred overnight and completion of reaction was confirmed by the TLC in ethyl acetate. NaCl solution and ethylacetate were added to the reaction mixture. The aqueous layer was discarded while the organic layer was rota evaporated to obtain the final products. Due to the continuous delocalization we expect electronic conduction in these novel compounds and the conductivity measurements are under progress. The absorption spectra (Fig.1) shows compound A exhibiting more delocalization than the other molecules, which could be possible due to the presence of the nitro group and hence red shift is observed. The infrared spectra (Fig. 2) show the corresponding two CN stretches indicating the di substituted products. In solution states compound A, B and C exhibit magenta Pink and yellow colored, leading to a chromophore effect.

PP-129

Ultrasonication assisted Michael addition reactions on 16- DPA molecule by use of intercalated Layered Double Hydroxides showing rehydrational 'memory effect'

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ABSTRACT

16-DPA (16-Dehydropregnenolone acetate) is an important intermediate for synthesising steroidal drugs with antitumour properties [1-2] and related other steroidal pharmacophores. Michael addition at C=C bond of D-ring position can be expected to give important molecules having application prospects in medicinal chemistry.Generally, Michael addition reactions are catalysed by basic catalysts like Na_2CO_3, K_2CO_3, alkyl amines, NaOH[3], potassium-tert-butoxide deposited on xonolite and KF deposited on alumina[4] Currently, Layered double hydroxides (LDH) are considered as important basic heterogenous catalysts as they are reusable, easily separable and environmentally benign[5]. Michael addition in D-ring of 16-DPA with malononitrile in presence of different calcined LDH- KF/K_2CO_3/Na_2CO_3/Cs_2CO_3 showed that faster addition takes place only if (1) the calcined LDH used can show so called 'memory effect', (2) the reaction is carried out under ultrasonication. XRD basal spacing change indicates that the reaction takes place in the confined interlayer space of LDH through intercalation of malononitrile and 16-DPA molecules.

PP-130
MICROWAVE ASSISTED SYNTHESIS OF A/D RING FUSED STEROIDAL PYRIMIDINES

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ABSTRACT
The steroidal heterocycles constitute one of the most interesting classes of organic compounds and their biological activities are well documented.[1] Pyrimidine and their derivatives are important constituents in nucleic acids, vitamins, coenzymes etc. which are vital to life processes. This heterocyclic moiety with biological and medicinal significance possess wide range of pharmacological applications such as antibacterial, anticonvulsant, antiprotozoal, antifungal, antiviral, antihypertensive, anti-inflammatory, antihistaminic activities.[2] In past few years various efforts have been made to annelate this pyrimidine moiety to steroidal heterocycles.[3] Amidines, the dinitrogen analogs of carboxylic acids and esters, display the combine properties of an azomethine like C-N double bond with an amide like C-N single bond having some partial double bond character.[4] Therefore, in continuation of our studies on the synthesis of azasteroids, [5,6] herein we report our recent results on microwave assisted synthesis of some A/D ring fused steroidal pyrimidines via cyclocondensation of steroidal bromoformyl system with amidine hydrochloride to form the steroidal fused pyrimidines. The newly prepared compounds will be further studied for their biological evaluation.

PP-131
Design, synthesis and characterizations of some novel N-substituted-2-benzo[d]imidazolylpyrimido[2, 1-b]thiazines for their biological activity

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ABSTRACT
Parasitic disease remains a major health problem particularly in the tropical developing countries. It is due to the treatment failure having occurred due to the development of the drug resistant parasites as available drugs have their limited pharmacological efficacy. Pyrimidines have displayed diverse pharmacological activities and play a vital role in medicinal chemistry as these are attributed to their ability to interfere against several important biological targets. Keeping in view importance of pyrimidines in parasitic area [1-4], a series of some novel some novel N-substituted-2-benzo[d]imidazolylpyrimido [2,1-b] thiazines were synthesized for their antiparasitic potency and the synthesized compounds were characterized by their elemental and spectral data analysis. In this presentation, the detailed synthetic procedure, mechanisms of the reactions and characterizations of the synthesized compounds by their spectral data (^{1}H NMR, ^{13}C NMR, EIMS and IR) analysis will be discussed.

PP-132
Design, synthesis and anticancer activity evaluation of amides of naturally occurring naphthoquinones.

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ABSTRACT
The naphthoquinones plumbagin, juglone, lawsone and menadione were chosen for the study. Prasad *et. al.* [1] reported the cytotoxicity of novel plumbagin hydrazone derivative against breast cancer cells. The pyrano and furano derivatives of lawsone with potent cytotoxicity were reported by Ngampong *et. al.* [2]. Saad Shaaban *et. al*. [3] and Laurence *et. al.* [4] have synthesized new cytotoxic derivatives of plumbagin and juglone. Ham *et. al*. [5] has reported the anticancer activity of sulphur containing analogues of juglone and menadione. This inspired us to synthesize similar thio Michael adduct of plumbagin, juglone, lawsone and menadione. Novel amides of the thio Michael adduct with various neutral amino acids were synthesized. The amides were evaluated against HeLa cells using MTT assay method.

PP-133

Design, Synthesis and Study of Benzodiazepine-Mustard Conjugates as Potential Brain Antitumour Agents.

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ABSTRACT

Nitrogen mustard is the one of the most active and widely used alkylating anticancer agents for the treatment of all types of cancer including cervix, breast and prostate cancer. One of the main demerits of mustard drug is their hydrophilicity which doesnot allow the molecule to cross Blood-brain barrier and therefore make these drugs not of much clinical significance to patients suffering from brain cancer [1]. Various lipophilic 1,4-benzodiazepine derivatives such as diazepam and nitrazepam has been known for their therapeutic CNS activity which is due to their action on Peripheral Benzodiazepine Receptors (PBRs). These receptors are located on the outer membrane of mitochondria, and their density is increased in brain tumours. Thus, they may serve as a unique intracellular and selective target for antineoplastic agents [2]. Moreover recent study reveals that some benzodiazepines derivatives have antiproliferative activities [3].

The combination of two pharmacological entities in a single compound could be considered as a promising drug design strategy for site-specificity. So we conjugated mustard with CNS active benzodiazepines for targeted delivery of mustard across brain by synthetic methodology. The benzodiazepine-mustard conjugates are oily at room temperature and stable when stored at less than 0°C. Structures of all the synthesized compounds were confirmed by I.R., ^{1}H N.M.R. and Mass spectral studies. The *in vitro* chemical alkylation activity studies (NBP) of benzodiazepine-mustards were comparable to that of mechlorethamine as standard alkylating agent. The compounds were markedly active when subjected to *in vitro* biological evaluation using MTT colorimetric method against human cancer cell lines (A-549, U-87 MG, COLO 205 and IMR-32). The Absorption, Distribution, Metabolism, Excretion (ADME) and Toxicity (T) ADME properties of these analogs were also studied and analyzed using Qikprop 2.5 tool of Schrodinger software which indicates that they can be a potential candidates for the treatment of brain tumor.

PP-134

Synthesis and evaluation of 6-aryl-imidazo[1,2-b]pyridazine -3- sulphonamide & related compounds for tumor necrosis factor-alpha (TNF-?) production inhibitory activity

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ABSTRACT

Tumor necrosis factor-? (TNF-?) plays important roles in the pathology of inflammatory diseases such as rheumatoid arthritis (RA), psoriasis, inflammatory bowel disease and multiple sclerosis. TNF-? also stimulates the production of other pro-inflammatory cytokines such as IL-1 and IL-6, and also induces the activity of degradative enzymes such as the matrix metalloproteases (MMPs). In clinical trials, the monoclonal TNF-? antibodies, Remicade (infliximab), the soluble TNF p75 receptor fusion protein (TNFRp75:Fc) and Enbrel (etanercept) have been shown to be effective in the treatment of RA and Crohn's disease. But the use of these biological agents are associated with severe limitations (e.g., parenteral route of administration, high cost of therapy, risk of opportunistic infections, induction of allergic reactions, activation of latent tuberculosis, increased risk of cancer, risk for worsening congestive heart disease). Therefore, inhibition of TNF-? has lately attracted considerable attention as target for antirheumatic agents.

Our desire for such therapeutics prompted us to investigate small molecules, which will inhibit TNF-? production. We started the search for small molecules for TNF-? production/ release inhibitor by looking its promising potential. We screened 3 series of compounds for TNF-? inhibitory activity. Out of 3 series, 6-aryl-imidazo[1,2-b]pyridazine was a good start for lead generation. The various modifications lead to the improvement for TNF-? inhibition in the range of 0.3- 10 ?M in hPBMC assay. 3-Sulfonyl-4-arylpiperidine-4-carbonitrile moiety on imidazopyridazine showed better activity compared to the 3-(4-aryllpiperazin-1-yl)sulfonyl) in hPBMC assay. Compounds from this series demonstrating moderate inhibitory activity in the *in vivo* LPS-induced TNF-? production assay in BALB/c mice. The moderate *in vivo* TNF-? inhibitory activity of these compounds can be attributed, due to the inferior PK profile. Chemical modifications aimed towards overcoming these liabilities will be discussed.

PP-135

Microwave-assisted Synthesis of Imidazo[1,2-*a*]pyridin-3-yl)quinoxalinones

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ABSTRACT

Imidazo[1,2]heterocyclic scaffold has been considered as a privileged structure for drug discovery and thus constitute a part of several marketed drugs including the sedatives zolpidem and alpidem, olprinone used for the treatment of heart failure, and zolimidine which is used to treat peptic ulcers and gastroesophageal reflux disease. Also, quinoxalinones have been identified as platforms for diversity-oriented synthesis for drug related molecules possessing a wide variety of biological activities such as anti-inflammatory, antimicrobial, and antidiabetic activities.

Grygorenko and coworkers has recently reported the synthesis and application of imidazo[1,2]hetarylglyoxylates for the construction of various imidazole based fused heterocycles of biological importance including imidazo[1,2-a]pyridin-3-yl)quinoxalinones under classical conditions with long reaction times. [1] We have now developed microwave-assisted methodology for the synthesis of a series of imidazo[1,2-a]pyridin-3-yl)quinoxalinones from corresponding imidazo[1,2-a]pyridine *via* imidazo[1,2]pyridylglyoxylates; whereby the methodology offers tremendous advantages such as clean chemistry, reduction in reaction times, easy work up procedure over the traditional reported method. The detailed work and methodology will be presented in the conference.

PP-136

Red Fluorescent Protein (DsRed) transfected *Leishmania donovani*: its applications in drug screening

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ABSTRACT

Reporter genes have proved to be an excellent and promising tool for studying disease progression and have been widely used for *in vitro*, *in vivo* drug screening, high throughput screening, and whole-animal non-invasive imaging for parasites and for study of several aspects of host–parasite interactions. DsRed derived from coral *Discosoma* a newly discovered protein [3]. It is relatively less toxic to cells and stable to pH variation (pH 5-12). DsRed has a high quantum yield and is photostable; these characteristics make DsRed an ideal candidate for fluorescence imaging, particularly for multicolor experiments involving GFP and its variants [3][2]. So DsRed can be used as a live marker to monitor dynamic and real-time processes in living cells and whole organisms and can eventually be explored for chemotherapeutic assays [1]. Recent advancement in fluorescence microscopy and flow cytometry was utilized to develop *in vitro* assays for antileishmanial screening. *Leishmania* promastigotes expressing RFP from episomal p6.5 vectors showed a bright red fluorescence distributed throughout the cell, readily distinguishable from control (wild type) parasites.

Transfected *Leishmania donovani* obtained by electroporation in presence of appropriate DNA constructs and culturing in DMEM medium containing antibiotic Tunicamycin. The transfected parasites were selected with progressively increasing drug levels, a final concentration of 20 µg/ml.

Transfected *Leishmania* parasites was developed for *in vitro* screening system. The efficacy of various antileishmanial drugs viz. Miltefosine, Amphotericin B and Pentamidine was tested at different dose levels using flow cytometry. As expected significant antileishmanial efficacy of Miltefosine, Amphotericin B and Pentamidine was observed.

PP-137

Determination of polycyclic aromatic hydrocarbons in water and solid samples from the Bharalu river course of Guwahati city

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ABSTRACT

Polycyclic Aromatic Hydrocarbons (PAH) can arise in the environment mostly from anthropogenic activities related to Oil and Petroleum products, various Natural combustions, and domestic combustion sources. The distribution of PAHs in the soil and water samples of rural and urban areas of nearof Guwahati city were studied; The methodology involves the extraction of PAH's from water samples by solvent extraction with dichloromethane. Solid samples were ultrasonically extracted with acetone/hexane and the extract was cleaned up on a silica gel/alumina column. The concentrated and cleaned up extracts were analysed by HPLC on C_{18} columns using a gradient of acetonitrile /water as the mobile phase and fluorescence detector. According to observed molecular indices, PAHs concentration in the soil and water of this city seems to be originated both from the high temperature pyrolytic process as well as from the petrogenic source, indicating a mixed PAH input pattern. The aim is to provide an overview of current knowledge, so as to assess the need for future monitoring of PAHs and the present capability for their analysis .

PP-138

NEW ABCB1 INHIBITORS BY MOLECULAR DOCKING

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ABSTRACT

Docking methods are a powerful tool for *in silico* screening and drug lead generation and optimization. In this work we describe the construction and preliminary validation of a model for the synthesis of new ABCB1 inhibitors. The over-expression of the ABCB1 gene has been frequently associated with the onset of drug resistance in many tumor histotypes. Because of an unfavorable balance between pharmacological and toxic activities until now no drugs have reached clinical application. This prompted to the search for new active and less toxic molecules with such activity. Years ago, we started the analysis of different diltiazem-like compounds for their ability to compete for excretion with the typical target of ABCB1 activity doxorubicin, in multidrug-resistant A2780/DX3 cells.

On the basis of these results and lacking a crystal structure, we tried to design for homology a model of ABCB1 that we validated using the results of our previously analyzed ABCB1 inhibitors. We thus used it for designing new compounds identifying some chemical features, such as the *S* configuration, the presence of Br in position X of the benzene ring, and an alkyl chain of 6 C with an unsaturated bond that, applied to the compounds, caused an increased activity. Paradoxically, when these features were summarized in a single molecule, which would have maximally improved its activity, as actually previously forecasted by our docking model, we found a lower activity than expected.

In conclusion, our docking model of ABCB1, seems to reliably satisfy our need to forecast, on the basis of molecular structure, the inhibitory activity of diltiazem-like molecules on the ABCB1 transporter and to design new active compounds.

PP-139

Improved delivery coupled with enhanced safety through nanoemulsion system bearing Amphotericin B

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ABSTRACT

Amphotericin B (AmB) is a gold standard drug for leishmaniasis therapy, however limited by poor solubility and dose dependant toxicity. In present work, AmB loaded stable oil-in-water nanoemulsion (AmB-NE) was designed to improve delivery potential and, to decrease unwanted side effects. AmB-NE was prepared by a modified emulsification-solvent evaporation technique by sonication of the organic phase composed of methanolic solution of AmB, 10% (w/w) soyabean oil, 3% (w/w) soya lecithin and absolute ethanol with aqueous phase composed of 4% (w/w) tween 80, 2.25% (w/w) glycerol and water, using a probe sonicator. The physicochemical properties of AmB-NE were characterized and the effect of various parameters was studied as well. Consequently, optimized AmB-NE formulation with droplet size of 166.9±7.08 nm, polydispersity index of 0.206±0.08 and negative potential (-39.7±0.36 mV) along with 97.05±0.87% AmB encapsulation efficiency was obtained. The scanning electron microscopic image revealed nanometric size and near spherical morphology of NE droplets. An *in vitro* release study showed sustained AmB release compared to free AmB. Relatively, less average percentage of erythrocyte toxicity for AmB-NE was observed (3.61±0.5%) than free AmB (5.36±0.2%) at a concentration of 1 mg/ml and viscosity of AmB-NE was found to be 0.12 pascals at same concentration. AmB-NE exhibited good steric stability *in vitro* where soya lecithin content was found to be efficient in preventing their destabilization.
These observations from present study suggest that formulated NE could be used as a promising carrier for AmB in order to potentiate its encapsulation along with reduction in undesirable toxic profile.

PP-140

CRYSTAL CHEMISTRY OF IMMOBILIZATION OF DIVALENT SR IN CERAMIC MATRIX OF SODIUM ZIRCONIUM PHOSPHATES

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ABSTRACT

Sodium zirconium phosphate (NZP) is a potential material for immobilization of nuclear effluents. It was observed up to ~1.98 mol% (6.07 wt%), of strontium could be loaded into NZP formulations without significant changes of the three-dimensional framework structure(1-5). The crystal chemistry of $Na_{1-x}Sr_{x/2}Zr_2P_3O_{12}$ (x = 0.1-1.0) phases has been investigated using General Structure Analysis System programming(6-9). The SrNZP phases crystallize in the space group R-3c and Z = 6. Powder diffraction data have been subjected to Rietveld refinement to arrive at a satisfactory structural convergence of R-factors. The PO_4 stretching and bending vibrations in the Infra red (IR) region have been assigned. SEM and EDAX analysis provide evidence of Sr in the matrix.

PP-141

Synthesis and characterization of biodegradable polymer based on malonic acid

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ABSTRACT

Aliphatic polyamide based on malonic acid was synthesized by the condensation polymerization technique. The structure of synthesized polyamide was characterized by Fourier transform infra-red spectroscopic (FT-IR), proton nuclear magnetic resonance spectroscopic (^{1}H-NMR), elemental analysis. Viscosity of synthesized polymer was determined by using Ubbelohde viscometer. Thermal behavior [using Thermogravimetric analysis (TGA)] and biodegradation of polymer was also investigated. Biodegradation observation of polymer dependent on growth studies, polymer was used as growth substrate by bacteria and therefore it was biodegradable. This copolymer has the lowest crystallinity and this result suggest that degree of crystallinity has a strong influence on the enzymatic degradation rate.

PP-142

Dual wavelength RP-HPLC Method for Simultaneous Determination of Two Antispasmodic drugs: Application in Pharmaceutical and Human serum

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ABSTRACT

A reverse phase stability indicating HPLC method for simultaneous determination of two antispasmodic drugs in pharmaceutical dosage forms of parenteral (injectable) and in serum have been developed and validated. Mobile phase ingredients consists of Acetonitrile: Buffer: Sulfuric Acid 0.1M (50:50:0.3 v/v/v), flow rate 1.0 ml/min using a Hibar® µBondapak® ODS C18 column monitored at dual wavelength of 266nm and 205nm for PGD and TMP respectively. The drugs were subjected to stress conditions of hydrolysis (oxidation, base, acid and thermal degradation). Oxidation degraded the molecule drastically while there was not so much significant affect of other stress conditions. The calibration curve was linear with a correlation coefficient of more than 0.995 for both drugs. The drug recoveries fall in the range of 98.557% and 101.23% with 10pg/ml and 50pg/ml limit of detection and 30pg/ml and 150pg/ml limit of quantification for Phloroglucinol and Trimethyl phloroglucinol respectively. Method was validated in accordance to ICH guidelines and was applied successfully to quantify the amount of Trimethyl phloroglucinol and Phloroglucinol in bulk, injectable form and physiological fluid. Forced degradation studies proved the stability indicating abilities of the method.

PP-143

Removal of fluoride from potable water using effective nano-adsorbents

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ABSTRACT

A novel Mn-Zr oxide nano-adsorbent with high sorption capacity for fluoride was prepared through co-precipitation method. X-ray diffraction (XRD) analysis indicated the formation of solid solution by metal species entering metal oxide lattices. Fourier transform infrared (FT-IR) revealed that the hydroxyl groups on the adsorbent surface were involved in the sorption of fluoride. Both anion exchange and electrostatic interaction were involved in the sorption of fluoride on the metal-metal oxide adsorbent. Synthesized nanomaterial was also characterized by UV-visible, BET and Raman spectroscopy.

PP-144

Prevention of Oxidative Overstress: A Coordination Approach

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ABSTRACT

Radical Chemistry in biological systems is one of the most talked areas of research these days with lot of antioxidants being examined for delaying cell aging and cell damage. Copper and iron catalysed Fenton reactions are reported as the prime source for the generation of reactive oxygen species (ROS) which happen to be the main culprits for the oxidative damage to the cells. However tendency of species to complex either of these metal ions to a redox inactive state can offer a valuable resistance to the free radical generation within the cell.

The work under context discusses a novel approach of complexation of these metal ions as redox inactive complexes which restrain them to participate in Fenton type reactions and accordingly the generation of ROS is minimised. Acetonitrile, Bathocuproine, Bathophenanthroline, Neocuproine and Thiourea, were observed to efficiently prevent the oxidative damage while DMSO, Histidine and Mannitol did not show any remarkable effect in suppressing copper catalysed oxidation of a model protein Bovine Serum Albumin (BSA). Besides the reported ligand species the screening approach is being explored for the antioxidant assessment of newly reported or synthetically modified natural product isolates.

PP-145

Synthesis of some chiral derivatives of pyrazole dihydropyridines

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ABSTRACT

1,4-Dihydropyridines are important compounds in organic chemistry and biology. Their synthetic utility has been exploited in natural product synthesis, particularly in the field of alkaloids and pyridobenzoquinolizine systems. Dihydropyridines were first synthesized by ***A. Hantzsch*** in 1882 from acetoacetic esters, an aldehyde, and ammonia.[1] The 1,4-dihydropyridines are the most effective of the calcium antagonists or calcium channel blockers. They are valued not only for their pharmacological effect, but also as a tool for the investigation of the calcium channel, particularly since the discovery that this class also includes compounds that have exactly the opposite action profile and are known as calcium agonists. There are even instances in which this reversal of activity is found between enantiomers.[2] By viewing advantage and potential utility of dihydropyridines, we herein report the efficient asymmetric synthesis of DHP derivatives. In contrast to the techniques used previously[3] in our enantioselective Hantzsch variant the chirality information is introduced using two different ? -keto esters in equimolar ratio. The separation of respective enantiomers and calcium channel antagonist activity of the synthesised compounds is under progress.

PP-146

Studies on Atomic Spectroscopic Terms and Term Symbols of Non-equivalent Electrons of f^3 d^1 Configuration Using Russell- Saunders Coupling Scheme

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ABSTRACT

Russell-Saunders and j-j coupling schemes are important coupling schemes to calculate the terms and to assign the term symbols to the terms to the valence electrons of free atoms. The atomic term symbols provide the information about the energy of atomic valence electrons, total spin, total orbital angular momentum, total angular momentum and spectral and magnetic properties of atom. In this proposed work computation is done to analyze all the possible terms for the non-equivalent valence electrons of f^3 d^1 configuration manually and the term symbols are assigned to the terms by using Russell-Saunders coupling scheme. The possible microstates calculated for the non-equivalent electrons of f^3 d^1 configuration are 3640 and the total numbers of atomic spectroscopic terms determined from these microstates are 42 which are quintets (9-types), triplets (11-types) and singlet's (11-types). The ground state term determined for the non-equivalent electrons of f^3 d^1 configuration is quintet L (^{5}L) and the ground state is quintet L six ($^5L_6$).

PP-147

A new route to synthesis of a-C-branched densely functionalized cyclopentenones by Morita-Baylis-Hillman Chemistry

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ABSTRACT

The Morita-Baylis-Hillman (MBH) reaction has become one of the most frequently used carbon-carbon bond forming reaction during the last decade. It is basically a reaction between an aldehyde or ketone and an activated alkene or alkyne in the presence of a suitable Lewis acid or base as a promoter to give highly functionalized product generally known as MBH adducts.[1] The functionalities of MBH adducts and their derivatives make them appropriate precursors for strategic synthesis of several complex natural products or natural product like molecules.[2] Very recently, a highly diastereoselective C-2 hydroxyalkylation of sugar derived densely *O*-functionalized cyclohexenones with different aromatic aldehydes in the presence of diethylaluminium iodide (Et_2AlI) by utilizing MBH chemistry has been disclosed by our group.[3] Encouraged by this piece of work, we now explored the title reaction of highly *O*-functionalized cyclopentenone with 2-nitrobenzaldehyde by using Et_2AlI as a Lewis acid promoter to obtain the desired MBH adduct. Once the reaction condition was optimized, we wanted to explore the applicability of this enone as an activated alkene in Et2AlI mediated MBH reaction with various representative commercially available aldehydes. Thus, the title reaction of highly *O*-functionalized cyclopentenone with various aromatic aldehydes was carried out under similar reaction conditions. The respective adducts were obtained as the diastereomeric mixtures in good to moderate yields. The details of this work will be discussed.

PP-148

Properties of the low-lying electronic states of 2,4-pentadien-1-iminium ion and its N-substituted analogues

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ABSTRACT

Semiempirical-based CI (PM3/CI) and ab initio-based methods (RHF, GUGA-CI) are employed to study the low-lying electronic states of 2,4-pentadien-1-iminium cation and its N-substituted analogues with electron-donating (methyl, isopropyl) and electron-withdrawing (fluoromethyl, trifluoromethyl) groups on nitrogen. The global minima of their ground states (S_0) with respect to the dihedral angles (G_3, G_4) are obtained at (180^0, 180^0) conformations [1]. However, the planar structure of the S_1 state is not necessarily a minimum as all bonds are not having p-bonding character in this state anymore. This results in a barrierless process of one-bond flip (OBF) [2, 3] around a single bond (C-C) in the S_1 state which was originally a double bond (C=C) in the ground state. During this rotation, the S_1 state becomes stabilized, whereas the ground state energy increases. At a certain torsion angle their energies will match and a conical intersection (TICT CI) between these two surfaces takes place. Consequently, a radiationless transition occurs to the ground state. Increase in the +I and –I effect on nitrogen shifts the TICT conical intersection point away from the 90^0 (G_3 dihedral angle) value, when the G_4 value is kept fixed at 180^0. The S_1 state arises due to the HOMO? LUMO transition, while HOMO-1? LUMO and HOMO?^{2}? LUMO^2 transitions are responsible for the S_2 state (biradical species). Transition moment values of the allowed S_0($1A_g$ –like) ? S_1 ($2B_u$–like) transitions are approximately 7.5 D. The first excited states are having radiative lifetime values around 215 ps [1], except for the trifluoro-substituted analogue (~125 ps). The vertical excitation energy at the (180^0, 180^0) conformation between the S_0 and S_1 states of the 2,4-pentadieniminium cation is predicted to be 3.3 eV (375 nm), which increases with substituents having +I effect on nitrogen, and decreases in the case of fluoromethyl compounds (~2.8 eV). Thus, photochemical properties of these model compounds can be tuned by proper choice of substituents on the iminium nitrogen. Consequently, the enhanced or reduced photoisomerization processes may lead to some significant changes in the bio-optical activities of the corresponding retinal PSB analogues.

PP-149

Recycling factors for ribosome disassembly in the apicoplast and mitochondria of *Plasmodium falciparum*

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ABSTRACT

The apicoplast and mitochondria of the malaria parasite *Plasmodium falciparum* have generated immense interest as sites for drug intervention due to their prokaryotic origin and indispensability for parasite survival. Genomes of both organelles are actively translated and antibiotic-mediated translation inhibition is deleterious for parasite growth. In *P. falciparum*, the nuclear genome encodes two copies of a poorly conserved ribosome recycling factor (RRF) that mediates ribosomal splitting, a crucial step for continuous translation. The targeting of two RRF homologs, RRF1 and RRF2, to the apicoplast and mitochondria, respectively was established by transient transfection of GFP-fusion constructs. Recombinant RRF1 disassembled surrogate *E. coli* 70S ribosomes and polysomes in the presence of apicoplast-targeted EF-G and complemented *E. coli* RRF in the LJ14*frr*^{ts} mutant. RRF2 also exhibited ribosome recycling activity by splitting of *E. coli* 70S ribosomes but failed to complement the LJ14*frr*^{ts} mutant. Additionally RRF2 was capable of forming dimers, unlike any RRF characterized thus far. Disulphide bonds were implicated in dimerization of RRF2 as dimer to monomer conversion was observed in the presence of increasing concentrations of DTT. Molecular modeling and docking identified Cys138 as the residue likely to be involved in disulphide bond formation. Additional localization of RRF2 in the cytoplasm was observed by immune-fluorescence microscopy using anti-RRF2 antibody suggesting adjunct functions for this factor in the parasite. Although proteins comprising subunits of *P. falciparum* organellar ribosomes are predicted to differ from bacterial and mitoribosomal counterparts, our results indicate that the essential interactions required for recycling are conserved in parasite organelles.

PP-150

Spectroscopic and Magnetic Studies of 'Ship-in-a-Bottle' Ni(II) Schiff base Complexes in Zeolite Y

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ABSTRACT

Zeolites are crystalline aluminosilicate materials having 3D framework. This specific structural robustness of zeolite can be coupled with the reactivity of metal complexes to synthesize the heterogeneous catalyst and they, on other hand show structural and functional analogy with biological systems such as cytochrome 450, [1-3] and these hybrid catalysts offer the advantages of site isolation, shape selectivity, but the solution reactivity. In present study our aim is to identify the geometry adopted by Ni(II) complexes of Schiff base ligand like N,N'-Bis(salicylidene)ethylenediamine (Salen) and 5-Bromo Salen, under encapsulation due to steric constraints provided by guest framework. These "ship-in-a-bottle" complexes are synthesized by bringing the metal ion and ligand together within the supercage of zeolite-Y and once synthesized, the large metal-complex cannot come out without destroying guest framework.[4] Different techniques are used to characterize these coupled systems. Powder XRD pattern indicates the retention of integrity of host framework even after encapsulation and intensity reversal of particular peaks empirically revels the presence of large complex inside supercage void. [5-6] UV-Vis and IR spectroscopic data indicate the complexation in "free" and encapsulated states and observed shifts in the peak positions for the encapsulated complexes probably suggest the distortion in geometry from their 'free' state.[7]

Magnetic studies provide a platform to predict deformed geometry around the metal. Theoretical studies, SEM analysis offer better understanding.[8] On the basis of evidences the geometry adopted by the metal complex on encapsulation and effect of size of metal complex are explained and correlated with the functional modifications in heterogeneous system in terms of reactivity, selectivity.

PP-151

Design, synthesis and anticancer activity of novel bis(indolyl)-1,3,4-oxadiazoles

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ABSTRACT

Indole-based alkaloids are widely used in anticancer research [1]. In recent years, bis(indole)alkaloids, a new class of indole-based compounds isolated from the marine organisms, have been emerged as antitumor agents. As examples, Topsentins, Nortopsentin, Dragmacidins and Rhopaladins are some of the naturally occurring bis(indole)alkaloids consist of a five-/six-membered heterocyclic ring or linear chain between two indole moieties which are known for their interesting anticancer properties [2]. In view of immense biological significance of these alkaloids, indole derivatives have been used as a lead compound to identify novel and potent anticancer agents [3]. Recently, we have identified bis(indolyl)thiadiazoles and bis(indolyl)hydrazide-hydrazones as interesting cytotoxic agents [4]. As a part of our ongoing research to develop novel anticancer agents, we have prepared bis(indolyl)-1,3,4-oxadiazoles from hydrazide-hydrazones by incorporating 1,3,4-oxadiazole between two indole rings. To study the structure-activity relationship, we prepared a series of the bis(indolyl)-1,3,4-oxadiazole derivatives and evaluated their anti-cancer activity. The synthetic procedure and cytotoxicity results of bis(indolyl)-1,3,4-oxadiazoles will be presented in the conference.

PP-152

Synthesis and biological evaluation of some novel 1,4-dihydropyridines as potential anti-tubercular agents

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ABSTRACT

Recent studies showed that 1,4-dihydropyridine-3,5-dicarbamoyl derivatives with lipophilic groups have shown significant effect on anti-tubercular activity. In continuation to this, we have synthesized new derivatives of 1,4-dihydropyridines bearing carbmethoxy and carbethoxy group at C-3 and C-5 of the DHP ring. In addition, 1*H*-pyrazole ring is substitutes at C-4 position. These analogues were synthesized by multi-component Hantzsch reaction. Structures of the compounds were determined by IR, NMR, ^{13}C and Mass spectra. The *in vitro* anti-tubercular activity of compounds against *Mycobacterium tuberculosis* $H_{37}Rv$ was evaluated. The lowest minimum inhibitory concentration value, 0.02 µg/mL and SI >500, was found for dimethyl 1,4-dihydro-4-(3-(4-nitrophenyl)-1-phenyl-1*H*-pyrazol-4-yl)-2,6-dimethylpyridine-3,5-dicarboxylate **3f,** diethyl 1,4-dihydro-4-(3-(4-fluorophenyl)-1-phenyl-1*H*-pyrazol-4-yl)-2,6-dimethylpyridine-3,5-dicarboxylate **4c** and diethyl 1,4-dihydro-4-(3-(4-bromophenyl)-1-phenyl-1*H*-pyrazol-4-yl)-2,6-dimethylpyridine-3,5-dicarboxylate **4e** making them more potent than first line antitubercular drug isoniazid. In addition, these compounds exhibited relatively low cytotoxicity.

PP-153

Synthesis of *meso*-(4-cyanophenyl)porphyrins, their photophysical and DNA photocleavage studies

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ABSTRACT

Porphyrin is an attractive supramolecular scaffold for the production of functionalized molecular tapes or self-assemblies in organic or aqueous media [1]. Porphyrins have been widely studied in a variety of applications in the fields of materials chemistry, nanotechnology, biosensors, fluorescence imaging, catalysis and medicine, particularly in photodynamic therapy (PDT) [2-5]. Functional group transformations on periphery of porphyrins lead to significant changes in their absorption and emission characteristics, consequently their physico-chemical properties [6]. In continuation of our efforts to prepare novel functionalized porphyrins [7] we have synthesized 5-(4-cyanophenyl)porphyrin and studied their interactions with calf thymus DNA using UV-vis and fluorescent spectroscopies. Absorption studies on these porphyrins showed significant shift of the soret band in presence of ctDNA. In emission studies we found marked increase in fluorescence with increasing concentrations of ctDNA. The cationic 5-(4-cyanophenyl)-10,15,20-tripyridylporphyrin showed efficient DNA cleavage at 1.0 µM concentration. Synthesis, characterization and biological studies of 5-(4-cyanophenyl)porphyrins will be discussed in the presentation.

PP-154

Antifungal activity of hydroxytriazenes and their ternary complexes with Vanadium (V) and thiourea

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ABSTRACT

3-Hydroxy-3-m-chlorophenyl-1-(4-sulphonamidophenyl) triazene, 3-hydroxy-3-n-propyl-1-(4-sulphonamidophenyl)triazene, 3-hydroxy-3-isopropyl-1- (4-sulphonamidophenyl) triazene, 3-hydroxy-3-m-tolyl-1-p-chlorophenyl triazene, were synthesized and their antifungal activity was screened. It was observed that hydroxytriazenes showed inhibitory activity at 100, 200, 500, and 1000ppm against two fungi: *Candida albicans* and *Aspergilluss fumigates.* Thus the study has brought about a novel application of this class of analytical reagents as an emerging class of bioactive chemicals.

PP-155

Efficiency of Superparamagnetic Nano Iron Oxide loaded Poly (Acrylamide-co-Acrylic acid) Hydrogel in Uptaking Pb^{2+} ions from Water

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ABSTRACT

A novel adsorbent, super paramagnetic nano iron oxide loaded poly (acrylamide-co-acrylic acid) hydrogel (super paramagnetic PAA hydrogel), was employed for the removal of toxic lead ions from aqueous solution. The influence of pH, contact time, metal ion concentration, adsorbent dose and temperature on the sensitivity of the removal process was investigated. The synthesized copolymer was magnetized insitu and the size, structure and coating of magnetic nano particles were characterized by TEM, XRD and FTIR analysis respectively. The sorption data was analyzed and fitted to linearized adsorption isotherm of the Langmuir, Freundlich and Temkin equations respectively. This hydrogel has been found to be an efficient adsorbent for toxic Pb^{2+} ions removal from water (>98% removal) and could be regenerated efficiently (>99%).

PP-156

Bismuth triflate catalysed condensation of indole with acetone under different reaction conditions

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ABSTRACT

Indole is one of the most important and versatile moiety found in natural products, pharmaceuticals, agrochemicals and other synthetic compounds [1,2]_ENREF_3. Due to their diverse biological properties, structural modification of indole has attracted great attention of synthetic organic chemist in recent years. Condensation of acetone with indole is a very complex reaction and gives mixture of different. The reaction of indole with acetone in the presence of both mineral and Lewis acid has proved to be complex in nature due to the formation of wide variety products via cyclizative condensation [3,4].

Metals triflates have been used as efficient Lewis acid catalyst in various organic transformations. In continuation of our interest in metal triflates catalysed reactions [5], we herein, report bismuth triflate catalysed condensation of indole with acetone under different reaction conditions. When reaction of indole was carried out in excess acetone it resulted in formation of spiro-indole compound (**3**) in presence of $Bi(OTf)_3$, whereas with other Lewis acid bis(indolyl)methane was obtained as major product. The structure of the product depends on the reaction condition and the catalyst used.

PP-157

Synthesis and Characterization of Some New 4*H*-1,2,4-Triazole Derivatives as organic fluorescent materials and potent fungicidal agents

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ABSTRACT

Prompted by rapidly expanding applications of organic fluorescent materials for electroluminescence (EL), dyelasers, sensors, probes, and phototherapeutic agents, development of new fluorescent organic compounds with high functionality has been the subject of intense study for more than a decade.[1-4] Multi-component and domino reactions are efficient and effective methods in the sustainable and diversity-oriented synthesis of heterocycles and such reactions have attracted enormous interest in recent years.[5]

In continuation of our research work on heterocyclic synthesis [6-7], herein, we wish to report a multicomponent one-pot clean and solvent-free cyclocondensation reaction of aniline / amino acids and cyclic ketones / indole 2,3-dione with

thiosemicarbazide yielding triazole derivatives in high yields and shorter reaction time which are displaying good to excellent florescent property.
Thiosemicarbazide and its derivatives are an important class of synthetic compounds, having large variety of applications due to their wide spectrum of biological activities including antiviral and anti-tumoral activities as well as parasiticidal activity against Plasmodium falciparum and Plasmodium berghei. The 1,2,4-triazoles and their derivatives are found to be associated with various biological activities such as anticonvulsant,antifungal, anticancer, antiinflammatory and antibacterial properties. Also several compounds containing 1,2,4-triazole rings are well known as drugs. For example, fluconazole is used as an antimicrobial drug, while vorozole, letrozole and anastrozole are non-steroidal drugs used for the treatment of cancer.
The important biological activities of triazole derivatives impelled us to take up the synthesis of these new combinational heterocycles which are likely to have augmented diverse biological activity. The developed MCR may provide a valuable practical tool for the synthesis of novel physiologically active agents containing the title core fragment. All the newly synthesized compounds have been characterized by IR, ^{1}HNMR, ^{13}CNMR, Mass spectra, fluorescence study and also been screened for antimicrobial activity.

PP-158

Kinetics of the Oxidation of Substituted Benzyl Alcohols with Pyridinium Dichromate

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ABSTRACT
Pyridinium Dichromate (PDC) was synthesized by the reaction of pyridine with chromium(VI) trioxide. PDC structure was verified by IR. Pyridinium Dichromate (PDC) oxidizes benzyl alcohol and substituted benzyl alcohols have been studied in non aqueous medium and in the presence of acid to the corresponding aldehydes. The reaction was carried out under pseudo-first order condition. The reaction has unit dependence on each of the benzyl alcohol and PDC. Electron –releasing substituent on benzyl alcohol accelerate the rate of oxidation, whereas electron-withdrawing group retard the rate compared to the unsubstituted benzyl alcohol. The observed experimental data was used to rationalize the hydride ion transfer in the rate-determining step.

PP-159

SYNTHESIS OF A TRYPTOLIN-PYRROLOPYRIDINONE ANALOG BY A CONSEQUTIVE PROCESS: UGI-3CR / AZA DIELS-ALDER / PICTET-SPENGLER

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ABSTRACT
An organic reaction can be considered as multicomponent reaction (mcr) when three or mere reagents are successively combined [1], obtaining in a minimum of steps, products with high structural complexity, which incorporates the majority of the atoms that are present in the starting materials, for example, the reaction described by ugi [2]. the most important advantages of the mcr are both, the ease for obtaining structural diversity (dos) [3] and the rapidly efficient preparation of chemical libraries of compounds with great interest in medicinal chemistry [4]. the mcr are powerfully synthetic tools, mainly when they are subsequently combined with post-condensation [5] or post-functionalization [6] methodologies. As a background, recently in our research group, two methodologies based on mcr combined with subsequent post-condensation processes have been reported. in the first, a series of tetrahydroisoquinolin-pyrrolopyridinones was prepared by a sequence: ugi-3cr / aza diels-alder / pummerer [7]. in the second, a series of aza-analogs of natural alkaloid nuevamine was prepared by a sequence: ugi-3cr / aza diels-alder / pictet-spengler [8]. In this work, the rapid preparation of a linear pentaheterocyclic system of type tryptolin-pirrolopyridinone was described. Tryptamine (**1**), 2-thiophenylacetaldehyde (**2**) and the isocyanide (**3**) were sequentially combined by an ugi-3cr using scandium (iii) triflate as catalyst to afford the 5-amino-oxazole **4**. then, maleic anhydride (**5**) was *in situ* added to obtain the pyrrolo[3,4*b*]pyridine-5-one **6**, which was inmediatelly s-oxidized to afford the compound **7**. finally, a pictet-spengler cyclization was carried out to obtain the tryptolin-pyrrolopyridinone **8** with 15% of overall yield, *scheme 1*.

PP-160
SYNTHESIS OF FLUORINATED AZASPIRODIENONES BY A SEQUENTIAL UGI-5CR / RADICAL CYCLIZATIÓN PROCESS

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ABSTRACT
The introduction of fluorine atoms in nitrogen heterocyclic compounds has specially been valuable in the drug discovery process such as the great improvement of their metabolic stability, biological activity, lipophilicity, and bioavailability [1].
The azaspirocyclic cyclohexadienones have the 2-azaspiro[4,5]decane skeleton, which is found in a variety of natural and synthetic products. These compounds have a great interest in medicinal chemistry due to the fact that present activity as HIV-1 protease inhibitor, antiarthritic and antigastrin. The azaspirocyclic framework is also found in the natural products, spirostaphylotrichin A, and annosqualine [2].

PP-161
SYNTHESIS OF NITROGEN HETEROCYCLES BY MCR/PICTET-SPENGLER CYCLIZATION PROCESS

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ABSTRACT
Multicomponent reactions (MCR's) [1] have showed to be powerfully synthetic tools due to the fact that by their use, heterocyclic compounds with high molecular complexity and structural diversity can be prepared [2]. MCR combined with other post-condensation or post-functionalization processes increases their synthetic potential [3].
MCR was carried out under classical Ugi conditions obtaining good yields. Aldehyde and isocynide stereo-electronic nature does not have significant influence over reaction, except when formaldehyde 30% was used. This matter was solved using paraformaldehyde to increase the yield of the Pictet-Spengler reaction. Through proposed methodology was possible to generate several C-C, C-N y N-N bonds in tryptoline products only in two reaction steps with a tetrazole substituent. In general adducts and products are stable and majority of these were obtained as white solids.

PP-162
SYNTHESIS OF TETRAZOYL-CHROMONES OF INTEREST IN MEDICINAL CHEMISTRY VIA MCR-I PROCESS.

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ABSTRACT
Multicomponent reactions (MCR) are an important class of organic processes, in which three or more reagents are sequentially combined to obtain products containing the majority of atoms present in the starting materials. These reactions showed to be a powerful tool in organic synthesis to obtain heterocyclic compounds with high complexity and structural diversity with great interest in medicinal chemistry.[1] Chromones are a naturally occurring compounds that present interesting biological and pharmacological activities with low toxicity.[2] Tetrazoles are heterocycles that receive considerable attention due to the fact that are interesting building blocks and target structures in organic synthesis.[3] The presence of the two privileged heterocycles as tetrazole and chromone in the same molecule has rarely been reported.[4]
In this work, we focused on preparation of compounds having these two skeletons of interest based on the use of multicomponent reactions, because they are both, simple and effective method for synthesis of nitrogenated analogs of important natural and synthetic products.[5] (Scheme 1).

PP-163

SYNTHESIS AND Characterization of Parent, Desilicated Zirconium Introduced ZSM-5 to study its property

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ABSTRACT

Zeolite ZSM-5 was synthesized by using fume silica, sodium aluminate, sodium hydroxide, tetrapropyl ammonium bromide(TPABr) at definite proportion. A homogeneous mixture was formed then is transferred to an autoclaved and kept in oven for 17 hour at 273K. After synthesis it was characterized by X-ray diffraction(XRD), Scanning electron microscopy(SEM), Infrared spectroscopy (IR), Thermo gravimetric analysis(TGA) etc. Synthesized ZSM-5 is desilicated by using standard procedure. Then prepared the NH_4ZSM-5, HZSM-5. The ZrHZSM-5 was prepared by different amount of (0.2%,0.5% and 0.8%) zirconium after loading on HZSM-5. The synthesized materials used to study catalytic property and parent ZSM-5 used in biological activity.

PP-164

Computer Aided Drug Design and Synthesis of Focussed Heteroaryl Derivatives as GPCR Mediators in Diabetes

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ABSTRACT

Prevalence of type 2 diabetes has risen dramatically during recent decades and there is an urgent need of new approaches for disease prevention and treatment. Several G Protein-Coupled Receptors (GPCRs) expressed in pancreatic islets are involved in the regulation of islet function and hormone secretion, and are therefore potential targets for treatment of islet dysfunction. (Ahren B.**) Homology modelling** using Swiss model was done from the abundant sequence information to generate a reliable model of GPCRs; an alternative to the absence of crystal structure of these receptors. **Pharmacophore modelling** was performed on chemically diverse molecules of the reported agonists for GPR40, (Negoro Nobuyuki *et al*) GPR119 (Jason W *et al*) and GPR120 using DISCOtech module of SYBYL X 1.2. The highest scoring pharmacophore models were considered the best, having hydrogen bond donors, hydrogen bond acceptors, aromatic and hydrophobic regions. It was further refined with Genetic Algorithm Similarity Program (GASP).Virtual screening resulted various kinds of chemical scaffolds, which were further modified and **docked** with the aim to predict their proposed binding mode, resulting in further refined filter of chemical scaffolds out of these the best Heteroaryl systems, specifically the five membered pyrazole ring system are being explored. Out of these compounds some of the virtual structures were synthetically explored, and 3-[3-(4-methoxyphenyl)-4-(phenoxymethyl)-1H-pyrazol-1-yl] acetic acid derivative class of compounds has been **synthesized** taking into the account of sustainability and feasibility of the chemistry, which may act as a starting point for the in-house discovery program.

PP-165

Novel 4-aminoquinoline based hybrids with improved *in-vitro* and *in-vivo* activity

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ABSTRACT

Malaria is an age old deadly parasitic disease caused by protozoan parasites of the genus *Plasmodium* and is still epidemic in most part of the world especially in sub-Saharan Africa, Southeast Asia and South America. In fact, in terms of human suffering, malaria is the third most infectious disease after HIV and tuberculosis [1]. World Health Organization (WHO) report indicates 216 million cases of malaria with around 655000 deaths in 2010; the most affected being African children and pregnant women [2].

Malaria eradication efforts faltered in the 1960s, following the development of resistance strains of chloroquine, the best and most widely used drug for treating malaria, and since then it has been on the decline. To overcome the problem of drug resistance, the use of combination therapy as a multi-therapeutic strategy achieved limited success [3], and recently Meunier *et al* [4] has put forward the concept of hybrid molecules in anticipation that these kinds of molecules may overcome drug resistance problems. In hybrid molecules two or more pharmacophores are linked together covalently and it is believed hypothetically that these compounds act by inhibiting simultaneously two different conventional targets. Keeping these points in mind to explore the novel concept of developing hybrid molecules for malarial chemotherapy and in view of the excellent antimalarial activity exhibited by triazine and pyrimidine moieties, we have synthesized a series of 4-aminoquinoline-triazine (**1**), 4-aminoquinoline-triazole-triazine (**2**) and 4-aminoquinoline pyrimidine (**3**) based hybrid molecules and evaluated their *in-vitro* antimalarial activity against D6 (chloroquine-sensitive) and W2 (chloroquine-resistant) strains of *Plasmodium falciparum* [5-8]. Selected compounds were also screened for their *in-vivo* activity in a mouse model of *Plasmodium berghei.* Some of the tested compounds have shown potent antimalarial activity when compared to standard drug chloroquine and artemisinin.

PP-166

Marine Nitropyrrole Alkaloids – A novel anti-tubercular molecule

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ABSTRACT

Recent advances in pyrrole chemistry have largely attracted many scientists to develop novel pyrrole molecules against tuberculosis, virus and microbes. In an attempt to test the anti-tubercular and anti-bacterial activity of pyrroles, different novel derivatives of Nitropyrroles were synthesized based on molecular hybridization technique and tested for the same. Some derivatives showed promising anti-tubercular and anti-bacterial activity [1,2].

PP-167

Chiral Heterobimetallic Complexes Targeting DNA-Topoisomerase.

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ABSTRACT

Development of new therapeutic modulaties for cancer chemotherapy is the subject of immense interest owing to the fact that many present treatment regimes (platinum-based drugs) in chemotherapy have failed or fall short either in terms of efficiency or toxicity problems associated with them. Among the non-platinum complexes for metal based chemotherapy, copper and zinc complexes have been much explored due to the fact that both copper and zinc are bio-essential elements responsible for numerous bioactivities in living organism. New Chiral Schiff base ligand L, derived from the condensation reaction of L-valine, O-vanillin was synthesized and characterized. The mixed ligand complexes were prepared by using imidazole as secondary ligand. Both monometallic as well as heterobimetallic complexes were synthesized and characterized by various spectroscopic techniques viz, IR, ^{1}H, ^{13}C, ^{119}Sn, ESR and ESI-MS. The *in vitro* DNA binding studies of both the complexes with CT-DNA were carried out by employing different optical methods viz UV-vis, fluorescence and viscosity measurement. Furthermore, DNA cleavage activity of the complexes with pBR322 DNA was studied in a 5mM tris-HCl/50mM NaCl at pH 7.2 and it was observed that both complexes can efficiently cleave double stranded DNA. Both the comp lexes exhibited preferential selectivity towards minor groove of the DNA helix. Moreover, these complexes were tested for their antimicrobial activity, the results showed significantly good activity in comparison to standard drugs.

PP-168

New modulated design and synthesis of Quercetin–Cu^{II}–Sn^{IV}/Zn^{II}–Sn^{IV} scaffold for potential chemotherapeutic application: in vitro DNA binding profile, DNA cleavage pathway and Topo–I activity

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ABSTRACT

New molecular topologies Quercetin–Cu^{II}–Sn^{IV} and Zn^{II}–Sn^{IV} **1** and **2** were designed and synthesized to act as potential cancer chemotherapeutic agents. Their interaction with CT DNA by UV–vis and fluorescence spectroscopy was evaluated revealing electrostatic mode of binding. The intrinsic binding constant (K_b) for **1** and **2** complexes were calculated to be 6.7×10^5 and 3.5×10^5 M^{-1}, respectively showing that complex **1** has greater binding propensity for DNA. Quercetin complexes are capable of promoting DNA cleavage involving both single and double strand breaks. Therefore, cleavage pathway was ascertained by the reaction of **1** with pBR322 plasmid by gel electrophoretic assay. ROS such as $OH^{\bullet}$, H_2O_2 and $O2^{\bullet-}$ are the major metabolites responsible for chronic diseases such as cancer, respiratory disorders and HIV, diabetes etc, therefore eliminating ROS by molecular scaffold involving SOD enzymatic activity have emerged a potential to develop novel class of drugs. Therefore, in vitro superoxide dismutase activity of complex **1** was evaluated by using a xanthine/xanthine oxidase–NBTassay with an IC_{50} value of 2.26 μM. Furthermore complex **1** exhibited significant topoisomerase I inhibitory activity at low concentration of 30 μM.

PP-169

Green Tea Extract Suppresses Lead Acetate Induced Hemolytic Changes in Rat Erythrocytes

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ABSTRACT

Objective: To evaluate the protective effect of Green Tea extract on lead acetate induced erythrocyte hemolysis both in vitro and in vivo condition.

Methods: Isolated erythrocytes from rat were incubated with lead acetate alone or in combination with Green Tea extract (GTE) for 90 mins at 37° C. Hemolysis was evaluated by estimating the % of haemoglobin in the supernatant. For in vivo experiment rats were randomly divided into four groups (n=5) and given only water, 0.1% lead acetate in drinking water and 0.1% Lead acetate + GTE (50 or 100 $mgKg^{-1}$) continuously for 4 weeks. At the end of 4^{th} week, blood was collected and analyzed. Spleens from all animal groups were processed for histopathological and biochemical analysis.

Results: In vitro exposure of erythrocytes to lead acetate caused dose dependent increases in the extent of hemolysis which was significantly reduced by co treatment with green tea extract. Lead acetate treatment caused significant alteration of hematological profile including TEC, Hb, PCV and RC in rats, whereas GTE administration minimized these alterations caused by exposure to lead acetate. Spleen from lead acetate treated rats exhibited severe histopathological lesions, whereas in GTE treated rats the severity of splenic lesion was less. Lipid peroxidation, a marker of oxidative stress was significantly higher in erythrocytes and splenic tissue of lead acetate treated rats and GTE abrogated this effect.

Conclusion: The findings of the present study explain the beneficial effect of GTE supplementation in lead acetate induced hemolytic anaemia and subsequent histopathological effect on spleen of rat.

PP-170

PHYSICO-CHEMICAL STUDIES OF NON-IONIC SURFACTANT IN MIXED SOLVENTS

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ABSTRACT

Surfactants are the useful products of chemical industries because of their numerous applications like cleansing agents in laundry, agriculture food technology, pharmaceutical drugs [1], enhanced oil recovery, and as floatation agents in the beneficiation of ores. The physio-chemical properties of aqueous surfactant solutions are the important in understanding the aggregation behavior of surfactants as well as the liquid structural changes in these solutions. The critical micelle concentration, CMC values of non-ionic surfactant Brij-35 in aqueous and mixed solvent (water + ethylene glycol (EG) or propane 1,2-diol (P12D) or propane 1,3-diol (P13D) or diethylene glycol (DEG) or 1,3-dioxolone (1,3-diox) or glycerol (Gly) have been obtained from UV-VIS spectrophotometric technique, respectively at 298.15,308.15 and 318.15K at three mole fractions (x = 0.0345, 0.0674 and 0.0969) of co-solutes. The observed data have been employed to determine thermodynamic quantities [2-3] of micellization (ΔG^o_{mic}, ΔS^o_{mic} and ΔH^o_{mic}) and micellar transfer (ΔG^o_{tr}, ΔS^o_{tr} and ΔH^o_{tr}) from water to mixed solvent. It has been observed that ΔG^o_{mic} values for aqueous Brij-35 solution increases on mixing a co-solute. Positive values of ΔS^o_{mic} suggests that micellization has been favoured by entropy gain. A molar excess volume of water + co-solutes lends additional support to this conjecture. Further, the observed positive ΔG^o_{tr} infers the non-feasibility of the transfer of micelles from water to mixed solvent. Such transference for systems containing DEG, EG and P13D is opposed by larger endothermic ΔH^o_{tr} . However, in case of system containing 1,3-dioxolane or P12D or glycerol the transfer is predominatly opposed by larger entropy loss.

PP-171

A simple and efficient protocol for synthesis of 1,2-diarylnaphtho[2,1-b]furan using sequential hydroarylation/Heck-oxyarylation

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ABSTRACT

The benzofuran and naphthofuran are ubiquitous structural motif present in large number of natural products as well as pharmaceutically important unnatural compounds [1]. Due to their wide range of biological activities numerous synthetic methodologies have been developed for this class of compounds [2]. Nevertheless, despite the number of methods developed, the search for more general and versatile synthetic methods from readily available starting materials for these compounds continues to be an active area of research in organic chemistry.

Recently, two methods were reported for synthesis of benzofurans and napthofurans using transition metal catalyzed oxyarylation. The first method used palladium catalyzed Sonogashira colupling of terminal alkynes with 2-iodo/1-iodonaphthols followed by cyclization [2] and in second method 2-hyroxy-a-arylstyrene derivatives were cyclized in the presence of copper acetate, air and 8-hydroxyquinoline to give benzofurans and napthofurans [3]. Herein we disclose a novel protocol for the synthesis of 1,2-diarylnaphtho[2,1-b]furans using sequential hydroarylation and oxidative Heck-oxyarylation. Initially, reaction of 2-naphthols with alkynes in the presence of catalytic amount of $In(OTf)_3$ gave 2-hyroxy-a-arylstyrene derivatives which on further reaction with iodoarenes in presence of $Pd(OAc)_2$ resulted in formation of 1,2-diarylnaphtho[2,1-b]furans in excellent yield. The method is simple, uses readily available starting materials and gives good overall yield. The detailed experimental procedure will be presented in the poster.

PP-172
Generation of a Synthetic Library of Cyclohexane-diamine Derivatives as Potential Antimicrobial Agents

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ABSTRACT
The diamine class of compounds such as ethambutol (EMB) and SQ109 have received much attention for the synthesis of new derivatives as antitubercular drugs. SQ109 which is a second generation agent developed from the first line drug ethambutol is one of the most promising anti-TB drug candidates at the clinical trials stage. Bromhexine, another diamine based compound, is a semi-synthetic derivative of the natural alkaloid vasicine, isolated from the Indian shrub *Adhatoda vasica*. Bromhexin and its metabolite ambroxol, which structurally are *N*-alkyl benzylamine derivatives of cyclohexylamine, are widely used as mucolytic agents with a low level of associated toxicity and have a pH-dependent growth inhibitory effect on *M. tuberculosis*. As a part of our ongoing efforts towards the synthesis of novel antimycobacterial agents, we became interested to modify the bromhexine molecule and a library of symmetrical and unsymmetrical cyclohexane-1,2-diamine and C-(3-aminomethyl-cyclohexyl)-methylamine derivatives were synthesized and evaluated for their antitubercular activity. Some of the compounds showed potent activity against *M. tuberculosis* H37Rv without any hemolytic activity upto 512 µg/mL. The time-kill kinetics of two most active compounds was also studied and results indicate that both the compounds showed rapid killing of the *M. tuberculosis*. The MBC was close to the MIC confirming its bactericidal nature and the kinetics demonstrated a potent sterilizing effect under aerobic growth conditions.

PP-173
Polarographic study of 3-hydroxy-3-phenyl-1-(2,5-dichloro phenyl)triazene

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ABSTRACT
Polarographic Study of 3-hydroxy-3-phenyl-1-(2, 5-dichlorophenyl)triazene in the Britton-Robinson Buffer solution between the pH range 3.5 – 8.0 has been attempted. The reduction of present compound of dropping mercury electrode (d.m.e) is diffusion controlled in nature and is reversible process involving six electron process. An attempt has been made to explan mechanism of electrochemical reduction of the 3-Hydroxy-3-phenyl-1-(2,5-dichlorophenyl)triazene (HPDCT).

PP-174
Synthesis of Ionic Liquid-Supported Hypervalent Iodine Reagent and Application in Organic Synthesis

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ABSTRACT
The chemistry of hypervalent iodine compounds has experienced a rapid growth in last two decades due to their highly selective and mild oxidizing properties, and environment friendly character [1]. They are now routinely used in organic synthesis as reagents for the synthesis of complex organic compounds. Polymer-supported hypervalent reagents have been synthesized to overcome some of the disadvantages associated with the corresponding monomeric analogues [2]. Although, polymer-supported hypervalent reagents are very useful for various transformations; they often have lower reactivities than the monomeric analogues. Efforts have been devoted to develop simple, nonpolymeric hypervalent iodine compounds which show reactivities similar to those of monomeric analogues. Recently, imidazolium derivatives of (diacetoxyiodo)arenes [3] and [hydroxy(tosyloxy)iodo]arenes [4] were prepared and used for oxidation and a-tosylation, respectively. These ionic liquid-supported hypervalent iodine reagents allowed easy recovery and recycling of the reduced aryl iodides either by extraction into an ionic liquid phase or by simple filtration. In continuation of our interest in application of ionic liquids in organic synthesis [5], herein, we report a novel strategy to synthesize ionic liquid-supported analogue of HTIB (Scheme 1). The ionic liquid-supported [hydroxy(sulfoxy)iodo]arene was reacted with different ketones to generate ionic liquid-supported 2-oxo-2-aryl (alkyl)ethyl sulfonates. The ionic liquid-supported 2-oxo-2-aryl(alkyl)ethyl sulfonates where treated with different nucleophiles to synthesize a-substituted ketones in excellent yield. High purities, short reaction time and simple purification without the need of column chromatography are the salient feature of this methodology.

PP-175
Iodobenzene diacetate-mediated synthesis of 2-arylamino-1,3,4-oxadiazoles

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ABSTRACT

There has been continuous and considerable interest in the chemistry of hypervalent iodine reagents due to their low toxicity, high stability, ready availability and easy handling. They are known to undergo ligand exchange and ligand-ligand coupling reactions in analogy with transition metals. The 2-arylamino-1,3,4-oxadiazoles have been found to display a wide range of biological activities including antimicrobial, anti-inflammatory and anticancer agents [1]. They have also been extensively used as a pharmacophore in medicinal chemistry due to their involvement in hydrogen bond formation [2]. General preparations of 2-arylamino-oxadiazoles involve the cyclization of thiosemicarbazide using phosphorous oxychloride, concentrated sulphuric acid, tosyl chloride and Burgess reagents [3]. Most of these methods have several disadvantages such as handling of toxic reagents, elevated temperature and prolonged reaction time. Consequently, there is a need for an alternative procedure involving milder reaction conditions. In our efforts to develop relatively benign and efficient protocol [4] recently we have prepared several 2-arylamino-1,3,4-oxadiazoles in high yields from readily available thiosemicarbazides using relatively benign reagent, iodobenzene diacetate under solvent-free conditions. Synthetic and mechanistic details for the formation of 2-arylamino-1,3,4-oxadiazoles will be shared during the conference presentation.

PP-176
Synthesis of pyrimido [4, 5-*b*] quinoline derivatives *via* a three-component reaction in aqueous medium

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ABSTRACT

The importance of quinoline and its annelated derivatives are well recognized by synthetic and biological chemists [1]. Pyrimido [4,5-*b*]quinolines (also known as 5-deazaflavins, dF) are an important classes of annelated quinolines of biological importance [2]. It is structurally similar to the pyrimido[4,5-*b*]quinoxaline ring system of the naturally occurring flavins. Hantzsch 1, 4-dihydropyridines (1, 4-DHP) are an important class of compounds with vital medicinal value which are used for the treatment of cardiovascular disease, such as hypertension and angina pectoris. Thus, there is a continuous quest to comprehend these biological processes and synthesis of novel functionalized dihydropyridine derivatives [3]. Multicomponent reactions by virtue of their convergence have attracted considerable attention from the point of view of ideal synthesis . MCRs contribute to the requirements of an environmentally friendly process by reducing the number of synthetic steps, energy consumption and waste production [4]. An important aspect of green chemistry pertains to the elimination of volatile organic solvents or their replacement by non-flammable, non-volatile, non-toxic and inexpensive "green solvents" [5]. Water complies all these stringent requirements and therefore, the development of synthetically useful reactions in water is of considerable interest [6]. As part of our continued interest on synthesis of diverse heterocyclic compounds of biological significance [7], we report here the synthesis of benzo[*h*]pyrimido[4,5-*b*]quinoline *via* one-pot three component reaction in aqueous medium using environmentally benign and cheap p-Toluenesulfonic acid (PTSA) as catalyst (Scheme-1).

PP-177
Synthesis and DNA cleavage studies of *meso*-substituted porphyrin 1,3,4-oxadiazoles

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ABSTRACT

Porphyrins are an essential class of natural compounds that are ubiquitous in nature. They play an important role in biological processes such as oxygen transport, electron transfer and photosynthesis [1]. Their interesting properties also make them useful as catalysts [2], drug delivery systems [3], nonlinear optics and in photodynamic therapy as a medicine [4, 5]. In order to integrate porphyrins into biomimetic systems and tune their optical and redox properties, efficient methods for functionalizing the porphyrin core are constantly under investigation. Five-membered 1,3,4-oxadiazoles are an important class of heterocyclic compounds with broad range of biological activities including antibacterial, antimycobacterial and anticancer activities [6-8]. Due to immense biological significance of porphyrin appended heterocycles, we have synthesized several porphyrins containing 1,3,4-oxadiazole moiety on the meso-position. Detail synthesis and DNA cleavage studies of novel porphyrin oxadiazoles will be discussed in the presentation.

PP-178

A facile and efficient synthesis of 2-arylamino-5-(3'-indolyl)-1,3,4-oxadiazoles as cytotoxic agents

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ABSTRACT

Indoles represent a very important and unique class of fused five-membered heterocyclic compounds which are probably the most prevalent among other heterocyclic scaffolds broadly found in nature [1]. The indole ring system is incorporated into a vast number of structurally diverse biologically active natural and synthetic compounds which were found to display anticancer, anti-diabetic, anti-rheumatoidal, anti-oxidant, anti-viral properties [2]. In the recent past, several indole containing heterocycles with interesting activities have been isolated. For example, Labradorins, Camalexin, Pimprinine, Topsentin, Meridianins and their analogues have shown good anticancer activities [3-6]. With interesting biological properties of indolyl heterocycles, recently we have identified bis-(indolyl)-1,3,4-oxadiazoles, indolyl-1,3,4-oxadiazoles, bis-(indolyl)-1,2,4-thiadiazoles, 2-arylamino-5-(indolyl)-1,3,4-thiadiazoles and 4-(3'-indolyl)oxazole as novel anticancer agents. Encouraged by these observation and in continuation of our efforts to identify potent and selective anticancer agents we have prepared a series of novel 2-arylamino-5-(3'-indolyl)-1,3,4-oxadiazoles by cyclodesulfurisation of acylthiosemicarbazides and evaluated their cytotoxicity against a panel of cancer cell lines. Details about synthesis and cytotoxic studies will be discussed during the presentation.

PP-179

PHARMACOPHORE MODELING, VIRTUAL SCREENING, MOLECULAR DOCKING, SYNTHESIS AND IN-SILICO ADMET STUDIES OF CYCLIN-DEPENDENT KINASE-2 (CDK2) INHIBITORS AS POTENTIAL ANTICANCER AGENTS

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ABSTRACT

Cyclin-dependent kinases (CDKs) are serine/threonine protein kinases. CDK activity is increased in proliferative diseases such as cancer, owing to the frequent overexpression of cyclins. CDK2 inhibition essentially restrains uncontrolled cell proliferation [1]. In this research, pharmacophore modeling was performed on 10 different molecules using DISCOTECH module of Sybyl X1.2 [2]. Among generated models, first model was considered as the best having highest score and refined with GASP. Out of the four models generated, model with the highest score was considered as the best model which contains 5 features viz. 2 H-bond donor, 2 H-bond acceptor and 1 hydrophobic region. This model was used as a query for virtual screening in NCI database. A total number of 52326 molecules were obtained after Lipinski filtering. From the results of virtual screening with compounds having highest Q_{fit} value and knowledge based structure activity relationship study, various molecules with substituted pteridine moiety were designed and docked on co-crystal structure of CDK2 (PDB ID: 2R3I) to predict the binding orientation of drug candidates to their protein target using Indirubin and Flavopiridol as standard drugs. From this, few derivatives bearing pteridine moiety having comparable docking score were synthesized [3] and characterized by FTIR, ^{1}HNMR and Mass spectral data. Synthesized compounds were evaluated for anti-cancer activity on various cell lines. *In-silico* ADMET studies were carried out using OSIRIS property explorer showing good drug-like properties of designed and synthesized molecules. The designed compounds showed good potential to be CDK2 inhibitors.

PP-180
NOVEL DITHIOCARBAMATE ANALOGS OF PHOSPHOCHOLINE: AS SPERMICIDAL AGENTS

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ABSTRACT
Overpopulation is the biggest fret of present era. According to United States Census Bureau, the current estimation of global population is 6.93 billion and data from the World Resources Institute suggests that global population will be raised by 34% by 2050. The high number of unintended pregnancies (40%) indicate the requirement for novel, women-controlled techniques of need based contraceptives which are easy to use, self-administrable, safe and affordable. Family planning and the use of contraception is the answer of this problem. Spermicide is one of the best contraceptive method and there is need to develop a vaginal spermicide, which is non-irritating to vaginal tissue, and having microbicidal properties and work through a selective mode of action. Dithiocarbamate (DTC) group is a versatile pharmacohore in medicinal chemistry. Functionalization of the DTC moiety offers an attractive method for the generation of derivatives, which may constitute interesting medicinal and biological properties. In recent years, it has been realised by various researchers that the introduction of a carbamate functionality into various biologically active molecules which significantly increases their biological activities.
The above facts encouraged us to synthesSize novel spermicides. We designed a series of dithiocarbamate derivative of phosphocholine. 20 compounds were synthesized which irreversibly immobilized human sperm at 1% w/v concentration.

PP-181
Superparamagnetic Magnetite Microspheres Composed of Polyvinyl alcohol and Alginate as Novel Adsorbent for Removal of Safranin–O from Aqueous Solution

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ABSTRACT
Using superparamagnetic magne The adsorption of cationic dye Safranin–O from aqueous solution by batch method tite microspheres composed of polyvinyl alcohol and alginate as the novel adsorbent has been reported. The above adsorbent was characterized by XRD, TEM and FTIR microscopy. On the surface of the prepared microspheres various static and dynamic adsorption studies were performed with Safranin–O at fixed pH and ionic strength. The progress of reaction has been monitored spectrophotometrically. The adsorption data were applied to Langmuir, Freundlich and Tempkin isotherm equations and the dynamic nature of adsorption was quantified in terms of several kinetic constants like rate constant for adsorption (K_1)and Lagergreen rate constant(K_{ad}).Modeling results showed that the uptake Safranin–O proceeded by physical adsorption. The influence of various experimental parameters such as pH, time, amount of adsorbent, effect of initial dye concentration, effect of temperature, effect of salts were investigated on the adsorption of Safranin-O.

PP-182
Study of the Phenolic Content and Antioxidant Activity of Bran of some Traditional Rice Cultivars of North-East India

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ABSTRACT
Phenolic acids are widely distributed in plant kingdom as aromatic secondary metabolites (Qiu et al. [1]). Interest in phenolic acids stems from their biological roles as antioxidants and from their roles in food quality (Robbins [2]). They are known to exert various physiological effects in humans, such as preventing oxidative damage of lipid and low-density lipoproteins, inhibiting platelet aggregation, and reducing the risk of coronary heart disease and cancer (Tian et al. [3]). Cereals are an excellent source of phenolic acids. An important cereal is rice, the staple food of India. However, rice is generally consumed as white rice or polished rice and as such the phenolic content in it is significantly reduced as phenolics are mainly compartmentalized in the pericarp of the rice kernel (Walter and Marchesan [4]). Hence in this study, the phenolic content and antioxidant activities of methanolic extracts of bran of four different traditional rice cultivars of North-East India was examined. The extracts were analyzed using Folin-Ciocalteu method for total phenolic content while 1, 1-diphenyl 2-picryl hydrazyl (DPPH) free radical scavenging assay was used for antioxidant activity determination. The results indicated that the total phenolic content of the extracts of bran of the traditional rice cultivars of North-East India was in the range of 0.268-1.42g GAE/100g bran. The IC_{50} value for the scavenging of free radicals was in the range of 0.63-162µg/ml. These results suggest a positive correlation between phenolic content and antioxidant activity. Hence rice bran of North-East India can be used as a potent source of antioxidants and as health promoters.

PP-183

Binding of an indole alkaloid, vincristine to double stranded DNA: spectroscopic and computational study

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ABSTRACT

Vincristine is a chemotherapeutic drug, used in clinics for the treatment of various cancers via inhibiting the mitotic spindle formation. A number of small molecules bind directly and selectively to DNA, acting as chemotherapeutic agents by inhibiting replication, transcription or topoisomerase activity. The binding of Vincristine to nucleic acids is of great interest for the control of gene expression and other nucleic acid mediated processes. In the present study, we have studied the interaction of Vincristine with four DNA decamer sequences by fluorescence spectroscopy and computational method. These spectroscopic profiles of Vincristine bound to different DNA oligomers show nonspecific interaction with the purine-pyrimidine bases. This binding influence of the drug molecule resides in the electronic environment of purine-versus pyrimidine residues in the DNA binding site. In addition, docking study revealed the presence of van der Waal's forces facilitates the interaction between the Vincristine and the DNA. In this study, we have evaluated that the DNA binding constants obtained for Vincristine were in the range of 10^4-10^6 per mole.

PP-184

Role of India in Global Pharmaceutical Sector with Emphasis on USA

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ABSTRACT

India currently represents fraction of global pharmaceutical industry but has potential to grow its share. The United States is the world's largest single market for pharmaceutical products. Governments worldwide are seeking to curb their soaring prescription drug costs through greater use of generics including Europe. India's comparative advantages lie in its cost competitiveness and its reverse engineering experience. Western pharmaceutical companies are now outsourcing a wide range of activities. Many mid-level Indian producers can turn to contract manufacturing, outsourcing, contract research, contract clinical trials, or other tie-ins with MNCs. Indian companies could not survive as global players without significant R&D expenditures and capabilities. Regulatory reforms are required in India to encourage leading global players to continue and accelerate the outsourcing of their R&D activities. This is particularly urgent in the face of the strong competition from China. The Indian Pharmaceutical industry can gain benefit as patents on a number of blockbuster drugs and biologics are scheduled to expire over the next few years. There is need to invest in R&D as the market for biosimilars will grow sharply in the coming years. The aggressive ANDA Para IV filing strategy will be one of the key determinants for the success of Indian generic companies in US; such filling is very less now. India can become big player on the world stage by focusing on developing biosimilars, challenging IPRs on regulated markets, investing in R&D for proprietary NCEs.

PP-185

NANOSCALE FIBERS WITH ENHANCED SORPTION POTENTIAL FOR TOXIC METALS FROM AQUEOUS SOLUTION

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ABSTRACT

in recent decades the development of selective and sensitive sensors and analytical procedures for the analysis of trace heavy metals has continued due to the great demand for the quantification of pollutants at lower and lower concentration levels in environmental and biological samples. different modified carbon paste electrodes have been used for the determination of metals including crown ethers, polymer films and enzymes. in view of safe and environment friendly modifier plant phytochemicals seem to play an important role. in this communication we report a totally environment friendly voltammetric stripping technique for the determination of lead and cadmium ions using a nano cellulosic fibers modified electrode. nano cellulosic fibers (ncfs) were prepared using physico-chemical treatment of rice straw, characterized using sem, tem, xrd and

explored for the determination of toxic metals from waste water [wang et al.]. tem micrograph of nano fibers, consisting of long and curved elongated nanoparticles with high length (micrometer scale) and low diameter (40–80 nm). modified electrodes were prepared by mixing of graphite powder and nanofibers with mineral oil using mortar and pestle. anodic stripping voltammetry in differential pulse mode was performed for the voltammetric analysis of lead and cadmium ions. different experimental and instrumental parameters were optimized for determination of these metals. the effect of interference and surfactants has been studied. the cheap, nonpoisonous modified sensor can be used instead of the severe toxic, expensive mercury electrode in this method. thus, it has excellent environmental and economical benefit.

PP-186

Comprehensive chemo-profiling of leaf and root extract of *Withania somnifera* using high-throughput multiplex approach of GC-MS, HPLC-PDA, 1D and 2D NMR.

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ABSTRACT

Withania somnifera (L.) Dunal (Solanaceae) usually known as Ashwagandha/Indian ginseng/winter cherry, is one of the most esteemed medicinal plants used in Indian System of Ayurveda for over 3000 years. It is used as herbal medicine for all age groups of patients without any side effects. The extracts as well as different isolated bioactive constituents of *W. somnifera* have been reported to possess adaptogenic, anticancer, anti-convulsant, immunomodulatory, antioxidative and neurological effects. The plant is also considered in the treatment of arthritis, geriatric, behavioural and stress related problems.

Herbal extracts represent combinatorial chemistry of nature with vast array of chemical ingredients that can deal with multiple targets (receptor) simultaneously leading to synergistic systems effect in order to demonstrate therapeutic benefit. Hence, instead of tracking a few marker compounds, comprehensive phytochemical fingerprinting is essential not only to ensure the quality of herbal medicines but also to establish their mode of therapeutic action with the help of molecular pharmacology. In this study 1D and 2D NMR, HPLC–PDA, GC–MS techniques have been employed for rapid comprehensive chemo profiling of *W. somnifera*, (Ashwagandha) leaf and root extracts. Total of 62 major and minor primary and secondary metabolites from leaves and 48 from roots were explicitly identified. Twenty-nine of these were common to the two tissues. These included fatty acids, organic acids, amino acids, sugars and sterol based compounds (including eleven bioactive sterol–lactone molecules). Twenty-seven of the identified metabolites were quantified. Significant qualitative as well as quantitative differences between the leaf and root tissue particularly with respect to secondary metabolites were noticed during investigation.

PP-187

Synthesis of Some New Thioether derivatives of Quinoxaline as Potent Antimicrobial Agents

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ABSTRACT

Different thioether quinoxaline derivatives were synthesized by conventional method and it synthesized by replacing the chlorine at C-2 with thioether linkage .The antimicrobial activity was assayed by agar plate disc diffusion method .Structure of the synthesized heterocyclic derivatives were confirmed on the basis of 1H NMR and FT-IR spectral data.

PP-188

Synthesis and biological evaluations of curcumin derivatives as possible microbicidal spermicides

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ABSTRACT

Curcumin, a hydrophobic polyphenol derived from the rhizome of *Curcuma longa*, possesses a wide spectrum of biological and pharmacological activities[1]. Curcumin has been found to show antioxidant, anti-inflammatory, antimicrobial, and anticancer activities. Additionally, curcumin has shown to possess the hepato and nephro-protective, myocardial infarction protective, thrombosis supressing, hypoglycemic, and antirheumatic effects. Apart from above mentioned activities, curcumin is also a poor spermicide. When curcumin is used in the concentrations of 300 µg/mL, 100% immobilization of spermatozoa was achieved.[2] Poor spermicidal activity of curcumin is due to its hydrophobic nature. Water solubility is essential for good spermicidal activity. Here, we are reporting an attempt to increase the water solubility of curcumin either by synthesising its amino alkyl derivatives or making its analogues containing tertiary amino group. These compounds were converted to water soluble tartarte salt before screening for spermicidal and antimicrobial activity.

PP-189

SCREENING OF KERATINASE PRODUCING FUNGI AND THEIR ENZYMATIC ACTIVITY FROM POULTRY WASTE

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ABSTRACT

Keratins are the most abundant proteins in epithelial cells of vertebrates and represent the major constituents of skin and its appendages such as nail, hair, feather, and wool. World-wide poultry processing plants are producing millions of tons of feathers as waste products annually, which consist of approximately 90% of keratin. In the present study from the decaying poultry feather samples five types of indigenous fungi were isolated and their enzymatic activity was measured. Each one of these isolated fungi showed variation in their enzymatic activity in different methods. In tris -buffer method, we found the green colored fungi with highest activity and yellow-green colored fungi with least activity. In the tris -phosphate buffer method, we found white colored fungi with highest activity and light pink colored fungi with least activity. From the overall analysis, we found white colored fungi with optimal activity in all the three methods. In these five isolates we identified white colored fungi as *Rhizopus spp*. black colored fungi as *Aspergillus spp.* and yellow green colored fungi as *Mucor spp.*

PP-190

HISTOCHEMICAL DISTRIBUTION OF DEHYDROGENASES IN THE REPRODUCTIVE TISSUES OF AMPHISTOME A RUMINANT PARASITES OF SOUTHERN RAJASTHAN

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ABSTRACT

On the basis of biochemical and histochemical studies, it has been established that the amphistomes parasites of Southern Rajasthan, primarily utilize the Embden-Meyerhof pathway for carbon metabolism. In the majority of tissues of reproductive duct and glands of mature amphistomes, the activity for the enzymes localized was found to be stronger and widely distributed in comparison to that in immature. The histochemical differences between diverse enzyme activities are also not very great. The intensity of Succinate dehydrogenase (SDH) and Malate dehydrogenase (MDA) activity dominated over the rest of the dehydrogenases. In contrast, activity of Isocitrate dehydrogenase (IDH) and a-ketoglutrate dehydrogenase (a -KGD) was comparatively low, in mature amphistomes that proved a functional tricarboxylic acid cycle (TCA) (cycle mainly ananorabic) may be operative in these worms. The intense activity of dehydrogenases in muscular reporductive tissues such as reproductive ducts is significant. Such a high activity of various dehydrogenases provides circumstantial evidence for the presence of successful operation of TCA cycle. Unlike many species of trematodes, amphistomes do not need the oxygen for the tanning of their eggs; hence it appears that most of the oxygen is utilized by the worm to run the TCA cycle to provide extra energy for muscular contraction of reproductive ducts and to keep up the metabolism of accessory reproductive glands. Moderate activity of mitochondrial enzymes in accessory reproductive glands appears to be in conformity to their requirements; the glands also need extra energy for high turnover rates of the secretory material. As such dehydrogenises may be involved in keeping up the general metabolis m of the gland cells.

PP-191

Self-assembly of Renewable Nanos: Nanoarchitectures from Arjunolic and Glycyrrhetinic acids

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ABSTRACT

Triterpenoids, the C30 plant metabolites are large and structurally diverse molecules having varied rigid and flexible lengths. Computations carried out by us on sixty representative naturally occurring triterpenoids have established that all the triterpenoids are nanometer long. We have been successful in isolating arjunolic acid from Terminalia Arjuna and glycyrrhetinic acid from Glycyrrhiza Glabara. Both the triterpenoids are nano-sized 6-6-6-6-6 triterpenoids. Detailed self-assembly studies revealed that both the triterpenics acids self-assemble in different liquids affording self-assembled fibrillar networks and spherical objects of nano- to micorometer diameters. The alkyl chained esters of the nano-sized arjunolic acid could immobilize various organic solvents at low concentrations. The molecules self-assembled in organic media to form nano- to micro-sized spherical objects and helical nano-fibers with concomitant hardening of the media (Figure 1). The melting of a soft material could be observed visually by concomitant color change. Recent results from our laboratory will be presented.

PP-192

Effect of various extracts of *Ocimum Sanctum* leaves on carbohydrate regulatory enzymes in vitro

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ABSTRACT

Natural product offers great hopes in the identification of bioactive compounds and their development into drugs for the treatment of Diabetes. Based on this literature survey we have undertaken a research programme to isolate lead molecules from Indian medicinal plants that have been used in Ayurveda for treating Carbohydrate metabolising disorders. Dried, powdered leaves of *Ocimum Sanctum* were successively extracted with Pet Ethet (A), Acetone (B), Ethanol (C), Water (D). The present study was designed to investigate the effect of this various extracts on Carbohydrate regulatory enzymes i.e. glucoamylase and a- amylase.

PP-193

Synthesis of some new chloroslubstituted isoxazolines and their curative effect on induced hepatotoxicity in *albino* rat

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ABSTRACT

lorosubstituted 4-aroyal – 2-isoxazolines (2a-d) were synthesised by condensing Chlorosubstituted 3-aroylflavanones (1a-d) with hydroxylamine hydrochloride in DMSO containing a little piperidine and assayed these compounds (2a-d) on cythion induced activities in *albino* rats with special reference to blood serem (VLDL,LDL and HDL) hepatotoxicity.The effects of intraperitonial administration of 4-aroyal $-\Delta^2$-isoxazolines (100mg/kg body wt.) were studied on cythion induced blood serum hepatotoxicity . The blood serum VLDL,LDL and HDL were estimated in order to assess the liver functions by established procedures .Biochemical observations were supplemented with histological examination of liver section . It is evident from the results that the levels of serum lipoproteins were more altered in cythion treated animals than controls .There was small but significant decrease in the concentration of total serum lipid concentration in the VLDL ,LDL & HDL .However ,the altered lipoprotein concentration levels were restored to almost normalcy in 4-aroyal $-\Delta^2$-isoxazolines treated animals.

PP-194

CONVERGING FEATURES OF NNRTI AGAINST DIFFERENT HIV-1 RT STRAINS: AN EXPLORATION VIA CoMFA/ CoMSIA

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ABSTRACT

The current anti-retroviral therapy (ART) needs new concepts leading to the elimination of HIV-1, which is the causative agent of AIDS. Among different classes of anti-HIV-1 drugs, RT inhibitors are most effective and selective ones. However, the virus is fast developing resistance against most of the drugs, for example Nevirapine, Efavirenze and Delaviridine. Hence, there is an urgent need to design and develop new molecules with broad spectrum activity against multiple viral strains. As an attempt towards this objective the HIV-1 RT target requirements of wild and mutant strains K103N, Y181C and Y188L are investigated by making use of a dataset of 152 pyridon-2-one derivatives in CoMFA / CoMSIA directed 3D-QSAR approach. Here, the docked conformations of selected pyridon-2-one derivatives active against wild and mutant strains were used to develop the 3D-QSAR models to probe the binding pockets requirements of respective viral strains. The study has resulted in highly predictive models against all four stains (cross-validated Q^2>0.60, non-cross validated r^2>0.86, test set r^2>0.60). It has also suggested that steric, hydrophobic and/ or electrostatic fields have essentially contributed in explaining the HIV-1 RT inhibitory activity of these compounds. In the CoMFA / CoMSIA field contour map scenario, among the four stains the molecular requirements for inhibition against wild, K103N and Y181C appear to be near to each other. In these cases steric field is the dominating force followed by hydrophobic and electrostatic. However, in case of Y188L strain the dominating field appears to be the electrostatic followed by steric and hydrophobic. A balanced incorporation of these fields in the molecular design may lead to promising inhibitors against multiple viral strains.

PP-195

Synthesis, characterization and biological aspects of Schiff base complexes of ruthenium

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ABSTRACT

The synthetic route and spectroscopic studies of Ru(III) complexes of biologically potent ligand derived from benzaldehyde and semicarbazide hydrochloride in definite proportions (1:1) under microwave radiations. Azomethine group containing ligand and their complexes have been characterized by means of various physico-chemical techniques viz. molar conductance, magnetic, molecular weight determination and spectral studies (UV, IR, NMR). The analyses data revealed that ligand coordinated to metals Ru(III) via nitrogen and oxygen donor atoms for the complexes formation. The ligands and their complexes have been screened in vitro against a number of pathogenic bacteria to assess their growth inhibiting potential.

PP-196

Effects of Catchment Land Use on Water Chemistry and Biology of Freshwater Tropical Lakes of India

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ABSTRACT

Human activities have invariably altered the chemistry and biology of surface waters. Although such effects have been variously addressed globally, there are still a number of unresolved issues concerning the role of catchment land use in controlling water quality of dry land lakes of India. The present study is an effort in this direction. Of the two lakes considered in the present study, catchment of Lake Baghdara is relatively undisturbed woodland and lake Udaisagar is mainly human disturbed arable land.

Concentrations of total dissolved solids (TDS), dissolved organic carbon (DOC) and major nutrient ions (NO_3^- and PO_4^{3-}) were significantly higher in lake Udaisagar. Dissolved oxygen (DO) however, showed an opposite trend. Biological characteristics such as phytoplankton chlorophyll and productivity showed spatio- temporal synchrony with lake nutrients and DOC but asynchrony with dissolved oxygen. Dry season supported prolific growth of phytoplankton. However, this effect was more pronounced for Udaisagar characterized by agricultural catchment. The study suggests that changes in catchment land use from natural to arable land exert significant modifying influence on biology and chemistry of receiving waters. This has relevance for integrated lake basin management especially in dry regions of the country.

PP-197

Comparative study of the oxidation of Nitro Benzaldehydes and Benzaldehyde by Pyridinium Fluorochromate in Non-Aqueous Medium

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ABSTRACT

Comparative kinetic study of the oxidation of *ortho*- nitrobenzaldehyde (ONBA), *meta*- nitrobenzaldehyde (MNBA), *para*-nitrobenzaldehyde (PNBA) and benzaldehyde (BA) by pyridinium fluorochromate (PFC) have been investigated in N, N-dimethyl formamide (DMF) medium in the presence of toluene *para*-sulfonic acid (TsOH) at 303 K. The reaction follows first order kinetics each in PFC, benzaldehydes and TsOH. The rate of oxidation remains unaltered by the variation of $NaClO_4$ but addition of $MnSO_4$ decreases the rate. The stoichiometry of the reaction is 3:2 and the products of oxidation were corresponding nitro benzoic acids and Cr (III). Activation energy and various thermodynamic parameters were calculated. The reaction rate was found to increase with a decrease in the dielectric constant of the medium. The reaction does not induce polymerization of acrylonitrile i.e. absence of free radicals. The presence of electron-attracting nitro substituent in the benzaldehyde moiety decreases the rate of oxidation. The observed order of reactivity is BA > MNBA > PNBA > ONBA. On the basis of experimental findings a suitable mechanism and a rate law has been proposed.

PP-198

EFFECT OF SELECTED DIETARY COMBINATIONS ON THE IRON CONTENT AND ITS AVAILABILITY

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ABSTRACT

It is estimated that 2 billion people worldwide are iron deficient, including 1 billion people who have iron deficiency anaemia. Iron deficiency is a common nutritional deficiency in developing countries. In India 66.9 per cent of children below the age of 5 years and 66.7 per cent young girls have anaemia. Habitual low intake, vegetarianism etc. are the primary causes. About 91 per cent of total iron intake in a mixed India diet is in the non-heame iron form. Individual dietary inhibitory and enhancing factors exert a profound influence on iron absorption. The extent to which iron absorption responds to the presence of enhancers and inhibitors were studied in the present work as such information is crucial in the understanding of how modification in the dietary enhancers and inhibitors could improve iron status of the malnourished population. The effect of mango powder, lime juice, tomato, tamarind and tea on the amount of total and bioavailable iron was studied.

Results reveal that the total iron content increased on adding mango powder, lime juice and ripe tomato15.22, 8.44 and 5.05 per cent respectively. While the iron content decreased on addition of tamarind pulp and tea by 1.73 and 62.72 per cent respectively. The *in vitro* bioavailability of iron was also affected to a large extent. Mango powder, lime juice, ripe tomatoes and tamarind pulp was found to increase the bioavailability of iron by 60.29, 49.95, 44.78 and 39.61 per cent respectively. While, tea was found to drastically decrease the bioavailability of iron by 63.81 per cent. It can therefore, be concluded that dietary modifications could perhaps be used to address the needs of iron deficient population.

PP-199

Synthesis of ZnO Nanoparticles

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ABSTRACT

Zinc oxide (ZnO) is a unique material with a direct band gap (3.37eV) and large excitation binding energy of 60meV. ZnO nanoparticles can be prepared by different methods such as precipitation method, mechanical grinding, solvothermal method, sol gel method etc. Stable, OH free ZnO nanoparticles (NPs) was synthesized by hydrothermal method by varying the growth temperature and concentration of the precursors by Aneesh etal[1]. ZnO NPs was synthesized by precipitation the surfactant solution.In this method precursors are zinc acetate, Ammonium carbonate and polyethylene glycol by Meruvu etal[2]. Sol-gel method is novel chemical method for synthesis of metal oxide NPs. Rani etal [3] synthesized ZnO NPs by using zinc acetate dehydrate and triethnolamine as the precursor materials. Biological approach using milky latex of Calotropis procera has been used for the first time as a reducing material as well as surface stabilizing agent for the synthesis of spherical-shaped ZnO-NPs by Singh etal[4].

PP-200

SYNTHESIS AND ANTIBACTERIAL EVALUATION OF 1, 3, 4-OXADIAZOLE DERIVATIVES CONTAINING FURAN MOIETY

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ABSTRACT

In past few years, the number of cases of multidrug resistant bacterial infection is increasing at an alarming rate. The clinicians have become reliant on new antimicrobial agents for serious infections due to development of resistance to traditional agents. 1, 3, 4-oxadiazole are five member aromatic heterocycles with great utility in synthetic, medicinal, and material chemistry. The widespread use of 1, 3, 4-oxadiazoles as a scaffold in medicinal chemistry establishes this moiety as an important bioactive class of heterocycles Fuloria et al.[1]. In the present research work, we had synthesized new substituted 1, 3, 4-oxadiazole derivatives containing furan moiety. The main key intermediates N^1-(substituted benzylidene) -furan-2-carbohydrazides were synthesised by reaction of furan-2-carbohydrazides with different aromatic aldehydes in presence of catalytic amount of glacial acetic acid Singh et al.[2]. Reaction of key intermediates with acetic anhydride resulted in the formation of corresponding 1-(2-substituted-5-(furan-2-yl)-1, 3, 4-oxadiazole-3-(2H)-yl) ethanone analogues. The structures of the synthesized compounds were established by ^{1}H NMR, MASS and IR spectroscopy techniques. Compounds were evaluated for their *in vitro* antibacterial activities using gram +ve & gram –ve bacterial strain. Most of the synthesized compounds showed good activity against the selected bacterial strains. Structure Activity Relationship studies revealed that oxadiazole analogues having hydroxyl substituted phenyl ring as well as unsubstituted phenyl ring showed highest activity against selected gram +ve & gram –ve bacterial strains.

PP-201

Microwave assisted One-pot Synthesis of Spironaphthopyranopyrimidine in aqueous medium

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ABSTRACT

Green Chemistry emphasizes the development of environmentally benign chemical processes and technologies. Multi-Component Reactions (MCRs) have emerged as a powerful tool for delivering the molecular diversity needed in the combinatorial approaches for the preparation of bioactive heterocyclic compounds. MCRs comply with the principles of green chemistry and are effective in building highly functionalized small organic molecules.In the present study we employed microwave energy to synthesized spironaphthopyranopyrimidine because the potential application of microwave technology in organic synthesis is increasing rapidly owing to its reaction simplicity, reduced pollution and minimum reaction time providing a rapid access to large libraries of diverse small molecules. Also such processes avoid costly purification processes that are inherently more environmentally benign and atom economic. Designing of MCRs in water is another attractive area in green chemistry. The scope of this reaction was successfully extended by employing other reactive ketones to access the synthesis of corresponding derivatives.

PP-202

SALINITY MEASUREMENT OF GROUND WATER

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ABSTRACT

"JAL HAY TO KAL HAY" : This line shows importance of water, in terms of its purity. Due to increase in use of water, under ground water level is going down at serious level day by day. The problem of salinity increases with decrease in ground water level. We have carried out measurement of water samples of different areas of Bhavnagar and tried to point out salinity level in drinking water to throw red light towards our nature of wasting water. The parameter studied were temperature, pH, chloride, sulphate, total hardness, total alkalinity, turbidity, & TDS. The ionic concentration is expressed in mg/L.

PP-203

Pharmaceutical evaluation of Garlic leaf extracts for their effect on carbohydrate metabolizing enzymes in vitro.

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ABSTRACT

There has been enormous interest in the development of alternative medicines for Type II diabetes, specifically screening for phytochemicals with the ability to delay or prevent glucose absorption. Herbal remedies are considered convenient for management of diabetes due to their traditional acceptability and availability, low costs and lesser side effects. The aim of the present study was to provide in vitro evidence for potential inhibition of glucoamylase and a-amylase to generate a stronger biochemical rationale for further studies on the various extracts of *Allium Sativum* leaves. Among the evaluated extracts, the chloroform and ethyl acetate extracts of garlic leaves revealed remarkable inhibition of glucoamylase activity as compared to pet-ether and ethanol extracts. Whereas, ethyl acetate and ethanol extracts showed significant decrease in a- amy lase activity.

PP-204

Mild and environmentally benign synthesis of 1, 8-dioxo-octahydroxanthenes

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ABSTRACT

Heterocyclic systems are common structural motifs in many biologically active substances and natural products and therefore necessitate the design of newer and efficient protocols for their synthesis. In view of this, Multicomponent reactions (MCR's) act as an important tool that can be used to rapidly generate vast libraries of heterocycles. In recent years, green chemis try which focuses attention on providing alternative reaction routes involving environmentally benign catalyst, avoiding use of toxic reagents and large amount of solvents resulting in effective chemical transformations have revolutionized the modern organic chemistry. The xanthene scaffold is probably the most ubiquitous heterocyclic structure in natural products as which usually possess biological activities and have been used as versatile synthon because of the inherent activity of the pyran ring. In this context, we have developed an efficient protocol for the synthesis of 1, 8-dioxo -octahydroxanthenes via simple condensation of dimedone and aryl aldehydes using heteropolyacid as a mild and green catalyst. (Scheme1).

PP-205

Effect of isolated sterols from leaves of *Vinca Rosea* on glucoamylase

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ABSTRACT

Natural products play an important role in the discovery of leads for the development of drugs for treating human diseases. Vinca Rosea belonging to the family Apocynacaeae is known with various names all over the world and is a perennial flowering plant. In the present study, the effect of various fractions obtained from the methanolic extract of Vinca Rosea by column chromatography were evaluated on the activity of glucoamylase in vitro. The fraction comprising of Ergosterol, Stigmasterol and ß-sitosterol found potent activators of glucoamylase at various concentrations. Thus the isolation of the bioactive molecule from medicinal plants would be effective drug target for particular disease.

PP-206

3D QSAR AND HQSAR STUDY OF 2-NITROIMIDAZOOXAZINE DERIVATIVES AS DEAZAFLAVIN DEPENDANT NITROREDUCTASE (ddn) ACTIVATORS

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ABSTRACT

Deazaflavin-dependent nitroreductase (Ddn) is an important target in the treatment of tuberculosis.[1] In this study, a diverse set of 2-nitroimidazooxazine derivatives were aligned for CoMFA, CoMSIA and HQSAR analysis. Rigid body alignment and pharmacophoric alignment methods were compared to get the best results.[2] [Fig. 1a and 1b] The best CoMFA model was obtained with the internal validation value (q^2) of 0.578 and conventional coefficient (r^2) of 0.999 with rigid body alignment. Various CoMSIA models were generated with different combination of fields. Out of which, the best CoMSIA model was obtained with steric, hydrophobic and HBA fields.[3] CoMSIA model was cross validated and the cross validation co-efficient (q^2) value was found statistically satisfactory (0.514). Both the models were validated by external set of 18 compounds with satisfactory prediction value of (r^2_{pred}) 0.612 and 0.608, respectively. HQSAR cross validation coefficient value (q^2) of 0.639 and r^2 of 0.837 were obtained.[4] The 3D QSAR approach provides significant insights that can be used to design novel and potent Ddn activators.

PP-207

A Comparative spermicidal activity evaluation of different salts of disulfide ester derivative (DSE-37)

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ABSTRACT

Fertility control constitutes a global health issue, as overpopulation and unintended pregnancy [1] have both major personal and social impact. As the world's population continues to soar, contraception has become increasingly important. Currently all commercially available spermicidal [2] have detergent ingredients that disrupt cell membranes. The present study is the extraplotation of previous findings. it involve the synthesis of new seven different salt of DSE-37 with a view to see the effect of different salt on spermicidal activity and their safety profile towards cervico-vaginal epithelium, normal vaginal flora and physical properties. The ascorbate salt of DSE-37 was the most potent spermicidal agent that irreversibly immobilized 100% human sperm at MEC of 21.57µmol. the other salts were relatively less active than ascorbate salt, and immobilized human sperm at MEC ranging 22.88-52.19 µmol in sander Cramer assay. However, N-9 was least active among all the spermicides and exhibited equivalent spermicidal activity at MEC 162.33 µmol.

PP-208
Design, synthesis and evaluation of Thiazolyl-pyrazoline derivative as antimicrobial agent

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ABSTRACT
Heterocycles are abundant in nature and are of great significance to life because their structural subunits exist in many natural products as well as in pharmaceutics, dyes and many more compounds. Hence, they have attracted considerable attention in the design of biologically active molecules. The pyrazoline and thiazoline derivative are known for their broad spectrum pharmacological activities such as antitubercular, antibacterial, anti-inflammatory and antidiabetic. These observations have prompted us to design and synthesize new active molecules having benzimidazole containing thiazolyl-pyrazoline nucleus. Newly synthesized compounds were tested for antimicrobial activity.

PP-209
MW assisted one-pot three component reaction of indole derivatives using $InCl_3$ as catalyst

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ABSTRACT
Heterocyclic compounds play a most significant role in drugs and pharmaceutical industries. Indole nucleus is a prominent structural subunit present in many naturally occurring compounds that possess significant pharmacological and biological properties [1]. A number of indole derivatives having heterocycles at the 3-position have been obtained from nature with potential biological activity [2]. The synthesis of polyfunctionlized 4H-pyrans group is attractive to researchers as it is a constituent of various natural products [3]. The main attention in 4H-pyran group is due to its biological and pharmacological [4] activities. These compounds are used as anti-coagulants, anticancer agents, spasmolytics, anti-anaphylactic etc [5]. The essential need of chemical research during current days is the development of resource and environmentally benign processes in terms of sustainable chemistry. In this regard development of new solvent-free reactions [6], use of catalyst like Indium chloride[7], application of microwave (MW) technology as nonconventional heating source [8], and one-pot multi-component reactions (MCRs) [9] are gaining considerable interest in the scienti?c community and pharmaceutical industry.
As part of our continued interest on indole and synthesis of diverse heterocyclic compounds of biological significance [10], we report herein the synthesis of novel polyfunctionalised pyran of indole derivatives *via* MW assisted one-pot three component reaction using $InCl_3$ as catalyst (Scheme-1).

PP-210
Microwave-promoted and Lewis acid catalysed synthesis of steroidal A- and D-ring fused 4, 6-diarylpyridines

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ABSTRACT
Due to the widespread biological activities, steroids bearing heterocycles fused to the A- or D-ring of the steroid skeleton continue to attract much pharmaceutical interest [1]. Great efforts are being made to annelate steroidal moiety with pyrazole, isoxazole, pyridine, pyran, pyrrole or pyrimidine rings using various synthetic strategies for the remarkable importance of these heterosteroids from the pharmacological and synthetic viewpoints [2-3]. Among these annelated heterosteroids, the synthesis of A-and D-ring fused pyridines draw particular interest because of the inherent biological activities of these heterosteroids [4]. In view of the therapeutic importance of heterosteroids and in continuation of our interest towards development of newer strategy for A- and D-ring annelated heterosteroids [5], we have developed one novel way for the synthesis of new steroidal 4,6-diarylpyridines from steroidal 1,5-dicarbonyl compounds using microwave irradiation and Lewis acid as the catalyst.

PP-211
Ionic Liquid-supported Palladium Complex: An Efficient and Recyclable Catalyst for Suzuki Reaction

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ABSTRACT
Ionic liquids are well known for their remarkable chemical and physical properties. They have been used as alternatives to volatile organic solvents for organic synthesis in homogeneous as well as in biphasic reactions [1]. Ionic liquids not only show improved reaction rate, but also facilitate product recovery and have the potential for recyclability. Catalytic transformations have been successfully realized in ionic liquids [2].
The transition metal complexes are extensively used as catalyst for varied organic transformations. The C-C bond forming reactions are very effective and important reactions in organic synthesis [3]. These reactions have influenced multiple areas of science, from the fields of organic synthesis and medicinal chemistry, to materials science and polymer chemistry [4]. The metal catalysts used for these transformations do not have good recyclability and reusability. To overcome this limitation, we have successfully synthesized a novel ionic liquid-supported palladium complex and used it for the Suzuki coupling (Scheme-1). Short reaction time, simple workup and reuse of the catalyst even up to six cycles without much loss of activity are the main advantages of the protocol. Details of synthesis and characterization will be shown in main presentation.

PP-212
Study of Indian Patents in Organic Chemistry Field in recent years

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ABSTRACT
With the advent of World Trade Organisation (**WTO)** on January 1, 1995, modern world is marked by Globalisation and liberalization. WTO also marked the beginning of a distortion free multilateral trade among the economies of the World (Venkateshwarlu et al.), This happened due to reduction in the customs duty to 5%. India has to compete with other countries like U.S. in the world market Due to globalisation, there is increase in international competition. Multinational corporations (MNC's) are important factors in the processes of globalisation. The obvious question is how MNC's can compete with each other? This is possible through Research and Development (R & D). Research is protected through patents. Here the role of patents becomes significant in the development of a country. In the post WTO era, patents have assumed greater importance in the scientific research and development and is being regarded as more valuable than traditional asset. Therefore, the analysis of patent filings in different classes has become important. The present study attempts to analyse the pattern of Indian patents in the field of Organic Chemistry filed during the past ten years. The search is based on the International Patent Classification system. The data are analysed with respect to the resident/non-resident status of the applicants, number of claims, spatial distribution of the patents, distribution of patents with respect to the gap between filing and Request for Examination etc.

PP-213
Rational-based design and synthesis of novel functionalized biphenyls as potent antihyperglycemic agents

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ABSTRACT
Protein tyrosine phosphatase 1B (PTP-1B) is an enzyme that plays a critical role in down-regulating insulin signaling through dephosphorylation of the insulin receptor [1]. The development of small molecule PTP1B inhibitors has emerged as a rapidly growing area of investigation in medicinal chemistry [2]. For the last few years, our group is involved in the design and synthesis of new antihyperglycemic agents for the treatment of diabetes [3]. We reported the synthesis, molecular docking and PTP-1B inhibitory activity of novel dihydronapthofurans and dibenzofurans [4]. In continuation, the biphenyl skeleton was chosen for further studies on the basis of recent literature study, which reveals that compound containing biphenyl pharmacophore possess significant antihyperglycemic activity [5].The desired functionalized biphenyls were prepared through carbanion-induced ring transformation reactions [6] of 2*H*-pyran-2-ones under basic conditions at room temperature. Some of these biphenyls exhibited PTP-1B inhibitory activity and showed blood glucose lowering activity in SLM, STZ, STZ-S and *db/db* animal models. The synthesis, *in vitro* and *in vivo* biological activity of these compounds are being presented.

PP-214

Analytical Application of 3-Hydroxy-3-isopropyl-1-(4-sulphonamidophenyl) triazene in the Spectrophotometric Determination of Nickel (II)

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ABSTRACT

3-Hydroxy-3-isopropyl-1-(4-sulphonamidophenyl)triazene has been used for spectrophotometric determination of Nickel(II) at 395 nm. The pH range was observed between 6.7 to 7.3. The Beer's law is obeyed in the range $1x10^{-5}$ to $6x\ 10^{-5}$ M. The molar absorptivity and Sandell's sensitivity values are 7076 $dm^3\ mol^{-1}\ cm^{-1}$ and 8.29 ng cm^{-2}, respectively. The Nickel (II) has been determined successfully even in presence of upto 100 ppm of various interfering cations and anions. The reagent forms complex with iron at ratio of 1:2. The composition of complex were determined by Job's method and Mole ratio method of Yoe and Jones. The value of log ß found from two different methods were 9.46 and 9.43 respectively.

PP-215

Analytical Application of *p* – Bromophenylazo-bis-acetoxime in the Spectrophotometric Determination of Iron (III)

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ABSTRACT

p- Bromophenylazo-bis-acetoxime has been used for spectrophotometric determination of Iron (III) at 370 nm, keeping the pH between 3.5 to 4.5. The Beer's law is obeyed in the range $1x10^{-5}$ to $6x\ 10^{-5}$ M. The molar absorptivity and Sandell's sensitivity values are 1030 $dm^3\ mol^{-1}\ cm^{-1}$ and 54.22ng cm^{-2}, respectively. The method is useful even in the presence of several cations and anions. The reagent forms complex with iron at the ratio of 1:2. The composition of complex were determined by Job's method and Mole ratio method of Yoe and Jones. The value of log ß found from two different methods were 7.98 and 7.32 respectively.

PP-216

Gamma ray Spectrometric analysis of fly –ash samples of Coal fired Thermal Power Plants

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ABSTRACT

The two potential sites studied during Gamma ray analysis of radionuclides in fly ash samples are Suratgarh Super Thermal Power Station, Suratgarh and Guru Nanak Thermal Power Station, Bathinda.

The activities of Cs-137,K-40,Ra-226 and Th-232(Bq/Kg) are 17.9,98.6,29.0 and 120.8 respectively for Suratgarh Super Thermal Power Station and 25.6, 96.5,25.1 and 123.1 respectively for Bathinda Thermal Power Plant. The Absorbed Dose Rate (n Gy h^{-1}) obtained for Suratgarh Power Plant is 90.58 and for Bathinda Power Plant is 89.97. The Effective Dose Rate (m Sv y^{-1}) in case of former is 0.111074 and for latter is 0.11034. Radium Equivalent Activity (Ra_{eq}) and External Hazard Index (H_{ex}) are calculated for the byproducts to assess the radiation hazards arising due to the use of fly ash in dwelling purposes. The valve of Ra_{eq} (Bq/kg) and Hex for Surathgarh thermal power plant are 209.57 and 0.5657 respectively and for Bathinda thermal power plant are 208.5 and 0.56317 respectively. The obtained results are below safe use values.

PP-217

Ligand free CuI catalyzed amination of 2-(2-bromophenyl)H-imidazo[1,2-a]pyridines in ionic liquids

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ABSTRACT

Imidazo[1,2-*a*]pyridines are an important class of fused aza-heterocyclic compounds. They have received great attention of synthetic and medicinal chemists due to their pronounced biological activities. Imidazo[1,2-*a*]pyridine scaffold are present in range of pharmaceutical compounds with antimicrobial [1], antiviral [2], anti-cancer [3], antiprotozoal [4], ?-aminobutyric acid (GABA) inhibition [5], etc. properties. Several drug molecules such as alpidem, saripidem, nicopidem, zolpidem, zolimidine, olprinone and YM529 having imidazo[1,2-*a*]pyridine as nucleus are in market. In continuation of our research interest in imidazopyridines [6], herein, we report an efficient C-N coupling of 2-(2-bromophenyl)H-imidazo[1,2-a]pyridine with different amines (Scheme 1). To the best of our knowledge, this is the first report for the synthesis of *N*-(2-(H-imidazo[1,2-a]pyridin-2-yl)phenyl)benzenamine using ligand free CuI in ionic liquids. It was found that among different reaction media, ionic liquid gave the best yield. It is also worthy to mention that the best yields were obtained with cyclic amines like imidazole, pyrroles etc. followed by secondary amines like *N*-methylpiperazine, morpholine and diisopropylamine. Aromatic amines such as anilne gave very poor yield. Detailed experimental procedure and results will be presented in the poster.

PP-218

ESTIMATION OF POLONIUM CONTENTS IN SOIL AND PLANT SAMPLES IN UDAIPUR, RAJASTHAN

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ABSTRACT

The study was performed using alpha counting system at College of Science, Mohanlal Sukhadia University Udaipur, Rajasthan. Through the study, the observed ^{210}Po activity in plant and soil sample from different locations in Bhoio Ki Pancholi area ranges from 2.45-173.50 Bq kg^{-1} on dry weight basis. The daily and annual intake of ^{210}Po through water was also estimated and the mean value of 0.72 and 263.61 Bq, respectively, were observed. It is observed that the effective doses through water were higher than the World Health Organization recommended dose of 0.05 mSv/year. The polonium contents in soil samples are in the range of 2.45-173.50 Bq kg^{-1} on dry weight basis. In soil samples minimum polonium contents was observed in samples no. BS I-17S. Maximum polonium contents (173.50 Bq kg^{-1}) were observed in sample no. BS II-4S. This soil sample was collected from the farmer's field in which it was growing *Triticum aestivum.* At site BS I, *Jatropha curcas* showed the maximum polonium concentration (22.67 Bq/kg) (sample no. BS I-7P). Certain other plants with high concentrations of polonium were *Azadirachta indica, Tabernaemontana divaricata* & *Lantana camara*. Minimum polonium concentration was observed in *Calotropis procera* (0.36 Bq/kg). In plant samples polonium contents was observed in the range of 0.36-25.94 Bq kg^{-1}. The plants of site BS II were also found to concentrate quite high polonium concentration ranging 1.91-25.94 Bq kg^{-1}. Maximum polonium contents (25.94) was observed in sample no. BS II-16P .

PP-219

INVESTIGATION OF ADSORPTION BEHAVIOR OF A CATIONIC DYE SPECIES ONTO GRAPHENE OXIDE NANOSHEETS

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ABSTRACT

Pollution of water resources by various pollutants is nowadays a subject of global environmental issue. Among the different types of water pollutants, dye represents a major polluting group [1, 2]. Though a number of processes are available for dye removal from aqueous system, adsorption is getting special interest due to its high efficiency, cost effectiveness and simple operation process [3]. In this study, graphene oxide (GrO) has been used for the adsorption of methyl green, a cationic dye molecule from aqueous solution at different experimental conditions. GrO consist of single layered graphite structure decorated with a number of oxygen containing functionalities such as carboxyl, epoxy, ketone and hydroxyl groups which impart negative charge density to it in aqueous solution at a wide range of pH. Thus, graphene oxide can be predicted as a good adsorbent material for cationic species. GrO was synthesized from powder graphite by Hummers and Offman method [4] followed by exfoliation of the product by ultrasonication. The kinetics of adsorption study shows that the adsorption equilibrium was reached at 60 min and follows the pseudo second-order kinetics. The adsorption isotherm has been investigated in the pH range 4-9 at 25 ^{o}C. The equilibrium data was ?tted well to the Langmuir model. Various thermodynamic parameters such as the Gibbs free energy (?G), enthalpy (?H) and entropy (?S) change were calculated. Negative value of ?G indicates spontaneity of the adsorption process.

PP-220

Synthesis of novel 1,2,3-triazole derivatives through click chemistry and evaluation of their antibacterial and antifungal activity

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ABSTRACT

1,2,3-Triazoles are one of the important heterocyclic compounds with numerous applications in chemical synthesis, material science and biological science. The classical approach for the synthesis of 1,2,3-triazole involves Huisgen's 1,3-dipolar cycloaddition of azides and terminal alkynes. Introduction of copper-catalyzed azide-alkyne cycloaddition (CuAAC) a premier 'click chemistry' reaction for their easy and efficient synthesis has aroused great attention of scientists from different areas in triazole chemistry.

The bioisosteric replacement of 1,2,4-triazole with 1,2,3-triazole is an efficient way for the discovery and development of novel triazole drugs in medicinal chemistry. In recent years, compounds with 1,2,3-triazole motif have been found to be potent antibacterial, antifungal, antitubercular, antineoplasic and anti-HIV agents [1-3]. Due to their chemotherapeutic value 1,2,3-triazole derivatives may be considered as new entry to azole antifungal agents. Herein, we reported synthesis of novel 1,2,3-triazole derivatives through 'click chemistry'approach. The 1,3-dipolar cycloaddition reaction of *N*-propargylpiperazines **1** with *in-situ* generated a-azidoketones afforded 2-(((piperazin-1-yl)methyl)-1H-1,2,3-triazol-1-yl)-1-arylethanone **3**, which was then converted to 1-((1-(2-(aryloxy)-2-arylethyl)-1H-1,2,3-triazol-4-yl)methyl)piperazines **4** by reduction with sodium borohydride followed by benzylation (Scheme 1). These newly synthesized 1,2,3-triazole derivatives were characterized by analytical and spectral data. All the synthesized compounds were evaluated *in vitro* for their antibacterial and antifungal activity.

PP-221

Design, Synthesis and application of Cell Penetrating Oligomers(CPO's) for efficient cellular delivery[1]

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ABSTRACT

Cell penetrating peptide have proved to the efficient and powerful tools for the drug delivery across the cell membrane. Among the synthetic peptides, (R-X-R)-type of peptides [1] were found to be more efficient. The amide backbone of peptides has been replaced by unnatural carbamate [2], carbonate, urea [3] or triazole linkages to achieve variety of applications. Here, we replaced the amide backbone in $(RXR)_4$ type of peptides by a carbamate backbone and envisioned more flexibility, enzymatic stability and possibly optimum spatial arrangement of the guanidine moieties in the designed oligomers.

We have synthesized activated carbonate monomers and incorporated them efficiently in designed oligomers. The newly synthesized oligocarbamates were found of amphipathic nature from octanol-water partitioning experiments. Circular Dichroism analysis confirmed flexible and unstructured compare to their oligoamide counterpart.

In-vitro analysis of the oligocarbamates by FACS showed enhanced cellular uptake over the oligoamide counterpart. Uptake studies implied an energy-independent and possibly direct penetration through cell membrane as the major mode of cellular entry. Confocal microscopic studies showed the oligocarbamates to be majorly located in the cytoplasm.

To test the applicability of the synthesized oligocarbamates as drug carriers, various cargoes ranging from small molecule therapeutic tripeptide (covalent attachment) as well as high molecular weight cargoes like labelled siRNA (siGLO) and plasmid DNA (charge complexation) were efficiently transported into mammalian cells. The efficiency of these oligomers was found to be as good as the known tranfection reagent Lipofectamine2000™ however with their low cellular toxicity. These results make oligocarbamates very attractive as future drug delivery tools.

PP-222

Immunoscreening of Brugia malayi cDNA expression library for identification of diagnostic filarial antigen(s)

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ABSTRACT

Filariasis is a chronic debilitating disease affecting millions of people in the tropical and sub-tropical countries. Due to non-availability of human filarial parasite in sufficient quantities antigens from heterologous filarial parasites have been used for the diagnosis of human filariasis. However, use of crude antigenic preparations from heterologous filarial parasites gave false positive results due to the complex nature of these antigens and their cross-reactivity with other helminth parasites. Therefore, characterization of these antigens is essential in order to identify the diagnostically important antigens. In the present study, immunoscreening of *B. malayi* ?gt11 cDNA expression library was done using IgG fraction of polyclonal antibodies against purified *S. cervi* antigen and the cDNA clones identified were cloned and characterized. The *B. malayi* cDNA expression library was plated onto a lawn of *E. coli* (Y1090) and the plaques (pfu) that were recognized by the polyclonal antibody were tested in PCR. Twenty two positive cNDA clones were obtained after first round of immunoscreening and 17 positive cDNA clones after third round of immunoscreening. The cDNA clone were PCR amplified and agarose gel electrophoretic analysis of PCR product revealed 0.4, 0.6 and 0.7 Kb insert in cDNA clone-6, cDNA clone-16 and cDNA clone-17 respectively. The purified PCR products were cloned in pGEMT-Easy vector, sequenced and characterized.

PP-223

Induction of host protective Th1 type immune responses using Bis-triazines derivatives for the treatment of Indian visceral leishmaniasis

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ABSTRACT

Visceral leishmaniasis (VL) is caused by protozoan parasites of the genus Leishmania and transmitted by an insect vector, the female phlebotomine sandfly. VL is a major worldwide health problem, has a high morbidity and mortality rate, and is classified as an emerging and uncontrolled disease by the WHO. Available treatments are problematic due to toxicity, high cost and emerging drug resistance. The survival of parasite within macrophage depends upon the suppression of host protective Th1 type cytokines (IL-12, IFN-? and TNF) and expansion of parasite protective Th2 cytokines (IL-10 and TGF-ß). Therefore, re-activation of immune cells for the production of Th1 derived immunity could prove to be the most effective strategy to combat the existing limitations with antileishmanials.

A series of fourteen novel bis-triazines derivatives were synthesized and evaluated for their antileishmanial potential against L. donovani. When evaluated in vitro against intracellular amastigotes, thirteen compounds were displayed better activity compared to the standard antileishmanials, sodium stibogluconate and miltefosine in respect to IC_{50} ranging from 0.77 to 10.32µM. On the basis of selectivity index, compound 9 was identified as the most active analogue exhibiting significant in vivo (L. donovani/ hamster model at 50 mg/kg, i.p. dose for 5 days) efficacy of 70% inhibition in parasite multiplication. Further studies on production of Th1/Th2 cytokines in mouse macrophage cell line (J774.A-1) indicated that compound 9 has the potential to skew the T helper cells towards Th1 type immune responses as significant enhancement in Th1 cytokine level was witnessed.

PP-224

Development of doxorubicin containing Nanocapsules for treatment of Visceral Leishmaniasis

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ABSTRACT

Leishmania donovani is causative agent for visceral leishmaniasis (VL) or 'kala-azar' in Indian sub-continent. Pentavalent antimonials, Amphotericin B and Miltefosine are the main drugs used for treatment but their irregular effectiveness, emergence of resistance in parasites against them; have necessasitated the use of other alternative drugs(1).

Doxorubicin, an anthracycline antibiotic used for the chemotherapy of various human cancers, was found to have potential leishmanicidal activity, but cardiac toxicity associated with the drug restricts its use as an antileishmanial agent. Previously, different reports have shown that incorporation of doxorubicin in liposomes and microcapsules can increase the therapeutic index and reduce toxicity(2).

The layer-by-layer method was utilized to prepare Sodium Alginate coated Nanocapsules having a nanoemulsion core loaded with doxorubicin (NCs-DOX). This formulation was tested for antileishmanial activity in-vitro in intra macrophage amastigotes and in-vivo in Leishmania infected hamsters. This formulation was demonstrated to be less toxic than free drug as measured through cytotoxicity assay by MTT. Higher parasite inhibition was observed in-vitro and in-vivo for NCs-DOX in contrast with free doxorubicin. Also NCs-DOX induced more apoptosis than the free drug in promastigotes. Moreover, NCs-DOX treatment drastically decreased the expression of Th2 cytokines- TGF-b, IL-4 and IL-10 in infected hamster as compared to free drug.

Hence, the new formulation NCs-DOX exhibited improved therapeutic efficacy with no major side in hamsters and thereby ensuring safer use over time and is possibly a better substitution for antimonials or other anti- VL drugs which has limited use due to the resistance and toxicity concerns.

PP-225

Copper-catalyzed efficient synthesis of arylaminoporphyrins

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ABSTRACT

Recently, there has been remarkable progress in copper-catalysed cross coupling reactions in the construction of various nitrogen heterocycles. Considerable advances have been made in the copper-catalysed Ullmann coupling due to a large demand of *N*-arylated heterocycles in natural product synthesis, chemical biology and drug discovery [1, 2]. Identification of novel tetrapyrrolic macrocycles of specific utilities in photodynamic therapy, catalysis, electronics and solar-cell productions has become one of the important targets for several research groups [3]. Also a variety of synthetic porphyrins and their metalloderivatives have been explored as efficient model systems for many life processes [5]. For the modification of core porphyrin, approaches including 1,3-dipolar cycloaddition and electrocyclization reactions have been utilized [4]. Recently, we have prepared porphyrin appended heterocycles and studied their photophysical properties and DNA cleavage activities [6]. For further structural modification of porphyrin macrocycles, we have synthesized several arylaminoporphyrins using copper catalysed C-N bond formation reaction. Synthesis and characterization of arylamino porphyrins will be discussed in the poster presentation.

PP-226

Interference of Pyridine moiety & H_2O in formation of Amide-to-Amide Hydrogen Bonds: A Case Study on the Crystal Structures of *Mono*-pyridyl-*mono*-amidealkanes and *Bis*-pyridyl-*bis*-amidealkanes

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ABSTRACT

Understanding the relationship between molecule and supramolecule is most fundamental and an important aspect for successful design in crystal engineering.[1]This relationship can be established by the study of a group of crystal structures of compounds containing almost similar functionalities. Thus crystal structures of series of mono(pyridyl)amides[2(a)], N,N'-bis(pyridyl)alkanediamides (amides)[2(b)] and N,N'-bis(pyridylcarboxamido)alkane (reverse amides)[2(c)] are analyzed and compared in terms of hydrogen bond networks. The amide (HN-C=O) is functional group thus packing of lattice is because of amide-to-amide hydrogen bonds but this is troubled by pyridine moiety in molecule. All amides show the dependency on the interplanar angle between amide plane and pyridine plane in the formation of amide-to-amide hydrogen bonds. The interference of pyridyl groups in amide-to-amide hydrogen bonds was found to be more prominent in reverse amides than amides. From these studies, geometric criteria were evolved that the interplanar angle (*?*) between the aryl (Ar) plane and the amide planes should be above 20° to form amide-to-amide hydrogen bonds. Free water molecules present in crystal lattice of reverse amides & their monopyridyl analogue also showed their effect. The water molecules join the amide molecules into 2D layers *via* water molecules (N-H•••O_w and O_w-H•••O). These 2D layers are further packed via C-H•••N and C-H••• p interactions in an alternate fashion. One of these reverse amides found to form a 4-fold interpenetrated network with quartz topology *via* N-H•••N hydrogen bonds.

PP-227

Ionic liquid-supported sulfonyl hydrazine: A novel 'catch and release' reagent for synthesis of pyrazoles

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ABSTRACT

Ionic liquid have received considerable attention in organic synthesis because of their unique chemical and physical properties [1]. They have been termed as a 'designer solvent' as their physic-chemical properties can be fine tuned by varying the cation or anion. Functionalized ionic liquids (FILs) have ability to behave not only as a solvents, catalyst, reagent and scavengers [2], but they can also be used as soluble support in organic synthesis [3].

Pyrazoles are important heterocyclic compound with a wide range of biological activities such as anti-inflammatory, anti-tumor, anti-mycobacterial, anti-analgesic and platelet aggregation inhibition [4]. In continuation of our interest in application of ionic liquids in organic synthesis, herein we report synthesis of ionic liquid-supported sulfonyl hydrazine as a novel 'catch and release' reagent and its application for an expeditious synthesis of pyrazoles (Scheme 1). The reaction of ionic liquid-supported sulfonyl hydrazine with unsaturated carbonyl compounds gives corresponding pyrazoles in excellent yield (76-89%). In an alternative approach reaction of ionic liquid-supported sulfonyl hydrazine with alkynes was also studied for synthesis of pyrazoles. High purities, excellent yield, short reaction time and simple purification without the need of column chromatography are the salient feature of this methodology. The method has advantage of both solid phase and solution phase synthesis.

PP-228

Antigenic analysis of embryo stage of *Setaria cervi*, the bovine filarial parasite

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ABSTRACT

Filariasis is a chronic debilitating disease affecting millions of people worldwide. Specific diagnosis and control measures are essentially required for effective control and management of the disease. It has been shown earlier that the excretory-secretory products (diagnostically important antigens) contain egg/embryo antigens, therefore, it would be important to characterize the embryo stage antigens for identifying the antigens having diagnostic potential. In the present study efforts were made to isolate and purify the embryo stage of *Setaria cervi* (bovine filarial parasite), produce polyclonal antibodies and analyse their protein and antigenic makeup. The *S. cervi* embryos (ScEmb) were isolated by dissecting gravid adult females and purification on two step Percoll gradient. The polyclonal antibodies were produced by immunizing the rabbits with ScEmb antigen. The SDS-polyacrylamide gel electrophoresis and immunoblotting analysis, using anti-ScEmb polyclonal antibodies, showed simpler protein and antigenic profiles of *S. cervi* embryo stage as compared to adult and microfilariae stage. The *S. cervi* embryo also showed high reactivity with the antibodies present in filarial patients sera thereby suggest the presence of some antigens common/cross-reactive with human filarial parasites. These studies demonstrate less complex nature of embryo stage of *S. cervi* as compared to adult and microfilarial stages and also reveal some qualitative and quantitative difference among three stages of *S. cervi*.

PP-229

Surfactant catalyzed unprecedented and greener synthesis of thia-azaspiro heterocycles in aqueous micelles

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ABSTRACT

Organic reactions in water without using harmful organic solvents have attracted a great deal of interest in both academic and industrial research, because in addition to environmental concerns there are beneficial effects of aqueous solvents on rates and selectivities of important organic transformations. Incorporation of surface-active agents (surfactants) in aqueous media has been proved to enhance the reactivity of water mediated reactions via the formation of micelles or vesicular cavities. The use of micellar and vesicle forming surfactants as catalysts in water is widespread and has been studied for a number of different synthetic transformations/ multicomponent reactions in water.

In continuation of our program to develop more efficient processes for the synthesis of biologically relevant sulfur and nitrogen containing heterocycles. Particularly intriguing is the spirocyclicooxindole scaffolds, which features in a large number of natural and synthetic compounds with important biological activities. Therefore, high speed, ultrasound-promoted, one-pot and multicomponent synthetic routes utilizing readily available reagents have been developed to produce a library of thia-azaspiroindole derivatives in water using surfactants for the first time. This new protocol produces novel heptacyclic spiro[indoline-3,4'-pyrazolo[3,4-e][1,4]thiazepine] dione derivatives in good yields via multicomponent methodology.

The regio- and stereo-selective compound has been confirmed by X-ray diffraction analysis. Detailed synthetic methodology and biological activities of these compounds will be presented in the conferences.

PP-230

A series of substituted malonamicacid thiosemicarbazide : An anti-tubercular agent.

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ABSTRACT

Tuberculosis remains the most important communicable disease in the world. Tuberculosis (TB) is an infection, primarily in the lungs (a pneumonia), caused by bacteria called *Mycobacterium tuberculosis*. Along with the recent increase in cases of tuberculosis, there is a progressive increase in multidrug resistant (MDR) tuberculosis. It was declared since 1993 by the World Health Organization (WHO), a global health emergency. Tuberculosis disease became a serious world-wide problem, particularly in people infected with the human immunodeficiency virus (HIV). At present, TB kills four people every minute some-where in the world and accounts about two million deaths per year. According to the WHO, currently one-third of world's population is infected with latent tuberculosis (WHO, 2006). Based on the trend over the past few years, a total of 225 million new cases and 79 million deaths are expected from tuberculosis between 1998 and 2030.

Therefore, we need to increase clinical importance of drug-resistant mycobacterial pathogens and has lent additional urgency to microbiological research and new anti-mycobacterial compound development. For this purpose, new malonamic acid thiosemicarbazide derivatives were synthesized and evaluated for anti-tubercular activity. Following compounds screened for anti-tubercular activity against $H_{37}Rv$ employing REMA (Resazurin microtitre assay) method. The structures were confirmed by their ^{1}H-NMR, IR and mass spectral data. Details of experimental procedure, purification, elemental and spectroscopic characterization methods will be presented during the meeting.

PP-231

Effects of Lactobacillus reuteri derived biosurfactant on gene expression profile of essential genes (gtfB, gtfC and ftf) in S. mutans adhesion

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ABSTRACT

The Streptococci are the pioneer strains in plaque formation and mutans Streptococci are the main etiological agent of dental plaque and caries. In general, biofilm formation is a step-wise process, which begins by adhesion of planktonic cells to the surfaces. Evidences show that expression of glucosyltransferase B & C (gtfB & gtfC) and fructosyltransferase (ftf) genes play critical role in initial adhesion of S mutans to the tooth surface which results in formation of dental plaques and consequently caries and other periodontal disease.

The aims of this study was to determine the effect of biosurfactants produced by probiotic strain; Lactobacillus reuteri (DSM20016) on gene expression profile of gftB/C and tft of S. mutans (ATCC35668) using quantitative real time PCR. .

The application of biosurfactant caused down regulation of the expression of all 3genes under study considerably. The reduction in gene expression was statistically very significant ($P>0.05$).

Therefre it is concluded that considerable down regulation of all genes in presence of biosurfactant is indicative of successful inhibitory effects of this probiotic products. In view of the importance of these gene products for S.mutans attachment to the tooth surface which is the initial important step in biofilm production and dental caries, therefore it is suggested that the biosurfactant prepared in this study is very successful in dental caries prevention.

PP-232

Effects of Lactobacillus reuteri derived biosurfactant on gene expression profile of essential genes (gtfB, gtfC and ftf) in S. mutans adhesion

*Ahmad Reza Salehi, **Rsoul Salehi, ***Gilda Eslami, ****Arezoo Tahmourespour, *****Omid Savabi

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ABSTRACT

The Streptococci are the pioneer strains in plaque formation and mutans Streptococci are the main etiolo gical agent of dental plaque and caries. In general, biofilm formation is a step-wise process, which begins by adhesion of planktonic cells to the surfaces. Evidences show that expression of glucosyltransferase B & C (gtfB & gtfC) and fructosyltransferase (ftf) genes play critical role in initial adhesion of S mutans to the tooth surface which results in formation of dental plaques and consequently caries and other periodontal disease.

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PP-233

Gene delivery to brain cells and glioblastoma cell line with apoprotein E derived peptide conjugated to polylysine (apoEdp-PLL)

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ABSTRACT

Gene therapy includes treatment of both genetic and non genetic diseases by transferring genetic material to the appropriate cells and organs. Viral or non-viral vectors are usually used to deliver desired DNA molecules to the target organ cells. Gene transfer using non-viral vectors are especially attractive because of their safety and low lmmunogenicity profiles. The existence of low density lipoprotein (LDL) receptors on the blood-brain barrier (BBB) provides an opportunity for non viral DNA delivery to the brain cells. Here we present the idea of using LDL receptor-mediated pathway for transporting genetic material to brain cells. A tandem dimer sequence of apoprotein-E (apoE) (141-150) conjugated to polylysine sequence was used as a novel DNA delivery vector for transfecting of brain cells either in vitro or in vivo.

The apoEdp-PLL vector is a 36 amino acid bi-functional synthetic peptide consisting of a 16 lysine chain at the amino terminus for electrostatic binding of DNA and the tandem dimer of apoEdp (141-150) 2 at the carboxyl terminus for binding to LDL receptor for transporting DNA across the BBB by using the LDL receptor mediated pathway.

pcDNA 3.1 and apoEdp-PLL were diluted separately in PBS. Solutions were mixed, vortexed immediately at a ratio of 1:8 (w/w) and left for 30 min at room temperature. Five μg of pCDNA3.1 complex with apoEdp-PLL vector was injected to the tail vein of female Balb/mic (5 weeks old). Animals were anesthetized after 48h and the dissected brain tissue was rapidly frozen in dry ice and preserved in liquid nitrogen until β-glycosidase staining. Control mice were injected only with 10μg PcDNA 3.1 and the brain tissue was frozen in similar way. Our findings suggest that capability of apoEdp-PLL for in vitro gene delivery to glioma cell line was more than 80%. In vivo administration of apoEdp-PLL delivery to brain cells after IV administration and X-Gal staining was found to be quite successful.

It is concluded that the synthetic apoEdp-PLL complex is a novel vector that acts efficiently for gene delivery to the brain cells.

PP-234

Cloning and sequence analysis of Lactate dehydrogenase from different strains of *Plasmodium knowlesi*

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ABSTRACT

Lactate dehydrogenase (LDH) is an important enzyme involved in the glycolytic pathway of malaria parasites. Higher vertebrates usually have different isoenzymic forms of LDH; however, *Plasmodium* possesses only one LDH isoenzyme. Genetic variation of the plasmodial LDH (pLDH) gene of different strains of malaria parasites has not been analyzed completely. In the present study, cloning and sequencing of LDH gene from different strains of *Plasmodium knowlesi*, the fifth human malaria parasite, was carried out to understand the genetic variation of the plasmodial LDH gene. The genomic DNA was isolated from infected monkey blood from two different strains (H and P) of *P. knowlesi* using QIAamp genomic DNA isolation Kit. The gene encoding parasite LDH was PCR amplified using genomic DNA and pLDH gene specific forward and reverse primers. The purified PCR products were ligated into EcoR1 site of pGEMT-Easy cloning vector and sequenced. The BLAST search program of NCBI was used for homology studies and the gene sequences were deposited in GenBank. Both *P. knowlesi*-H (PkH) and *P. knowlesi*-P (PkP) strains showed 951 base pair long LDH gene with same amino acid sequence. No difference was observed between the two strains of *P. knowlesi*. The BLAST analysis of the PkH and PkP strains gave 96% homology with *P. vivax* and 90% homology with *P. falciparum.*

PP-235

Synthesis and characterization of some new 1-substituted-3-methyl-4-(hydrazono)-2-pyrazolin-5-one

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ABSTRACT

Various 1-substituted-1,3-benzothiazole-2-yl) thiocarbamoyl-3-methyl-4-(substituted phenyl hydrazono)-2- pyrazolin -5-one have been synthesized by the reaction of ethyl 2-[(substituted phenyl) hydrazono]-3-oxobutanoate with substituted -1, 3-benzothiazole-2-yl-thiosemicarbazide. The structures of the all compounds have been established on the basis of IR and ^{1}H NMR and elemental analysis data. The evaluation of biological properties of the compounds is in progress.

PP-236

A Journey of Tissue Cultured Plants from Laboratory to Field andClonal Fidelity Analysis

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ABSTRACT

An efficient and rapid regeneration protocols of some medicinal plants viz., *Withaniasomnifera*, *Vitexnegundo*, *Phyllanthusamarus*, *T. indica* have been developed through different explants viz., nodal segments, intermodal segments, shoot tip etc. Proliferation of these differentiated tissues of diverse medicinal plantsmentioned was achieved on Murashige and Skoog (MS) medium supplemented with different concentrations of cytokinin and auxins. Multiple shoots of these plants were achieved on MS medium fortified with BAP, Kn and TDZ separately or in combinations. Elongation of these shoots was obtained after regular sub culturing on the same medium and growth hormones like Gibberellic acid. These shoots were detached from the shootclump and subcultured on rooting medium consisted with reduced strength of MS salts along with different concentrations and combinations of auxins (Indole 3- butyric acid, Naphthalene Acetic Acid). The *in vitro* recreated shoots were rooted best on half strength MS salts medium with Indole 3- butyric acid (0.5 mg/l to 1.5 mg/l). The complete plantlets have been transferred to small thermocol cups containing different potting mixture such as soil, vermi-compost, soil rite along with autoclaved garden soil (1:3) and coco-peat for hardening. Coco-peat gave maximum percentage of survival rate of the plantlets in the nature (90%). The hardened plants were used to validate the clonal fidelity through Inter simple sequence repeat (ISSR) markers in case of *Tylophoraindica*. The dendrogram based on the unweighted pair group method with arithmetic averaging (UPGMA) depicted about 93 % homology between the mother plant and micropropagated plants.

PP-237

Analysis of pharmacodynamic interactions between *Convolvulus pluricaulis* choisy. and available antidepressant drugs

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ABSTRACT

Mood disorders encompass a large group of psychiatric disorders and these are best characterized as syndromes rather than disease entities (Mitterauer, 2004). Since all the synthetic drugs available for the treatment of depression have various adverse effects people switch towards herbal drugs. The possibility of concomitant use of various antidepressants along with herbal drugs could not be overlooked. But use of herbal drugs is not always safe. *Convolvulus pluricaulis* has been reported to have antidepressant effect in animals and humans (Dhingra *et al.,* 2007). With this background pharmacodynamic interactions between and available antidepressant drugs were investigated in laboratory animals. Three different doses of *Convolvulus pluricaulis choisy* extract (CP) were administered along with different doses of antidepressant drugs viz. venlafexine, amitriptyline, fluoxetine and citlopram for 15 days. At the end of the treatments the animals were subjected to forced swim test and tail suspension test for assessment of depression and actophotometer and rota rod apparatus for assessment of neuromuscular toxicity. CP alone did not show any toxic effect in the doses tested. The combination of venlafexine, amitriptyline and CP did not show any interactions effects but a significant decrease in effectiveness of fluoxetine and citlopram were observed when administered along with CP.The study concludes that *Convolvulus pluricaulis* could not be considered a safe drug when taken along with synthetic antidepressants.

PP-238

Synthesis of trans dichlorotetravinylimidazoleruthenium(II) and trichlorodimethyl sulphoxide-S-(1,10-phenanthroline) ruthenium (III) complexes: Spectroscopic, Electrophoresis, Electrochemical and Theoretical studies on the CT- DNA binding and Biological studies.

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ABSTRACT

The ruthenium complexes of vinyl imidazole and -1,10-phenanthroline ligands, such as $[Ru(Vim)_6]Cl_2$ and $[Ru(phen)(DMSO)Cl_3]$ have been prepared. The compounds were characterized from the spectroscopic data and elemental analysis. The molecular structures of these compounds were determined by single crystal X-ray diffraction study. Binding of these complexes with calf thymus(CT) DNA was studied by UV-Visible and emission spectra. The electrophoresis and electrochemical studies have been performed to examine the CT-DNA binding of these complexes. The DNA binding features of theses complexes within cisplatin bonded region of DNA have been studied with molecular docking, MM and QM/MM studies. The anticancer activities of these compounds against Dalton's lymphoma (in vitro and in vivo) are also found significant.

PP-239

In vivo transformation of lung cells with apoprotein E derived peptide conjugated to polylysine (apoEdp-PLL): a non-viral vector for gene therapy

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ABSTRACT

Gene therapy is defined as the technology by which genes, small DNA or RNA molecules are delivered to human cells, tissues or organs to correct a genetic defect, or to provide new therapeutic functions for the ultimate purpose of preventing or treating

diseases. It is an exciting field of biomedicine that has the potential to benefit patients affected by particularly complex diseases like cancers. A wide range of viral and non-viral vectors have so far been used each with specific strengths and weaknesses, and numerous attempts have been made to overcome these hurdles in order to optimize gene therapy protocols. For diseases with challenging current treatment the innovative strategies like gene therapy is highly demanded.

Two diseases, cystic fibrosis (CF) and a_1-antitrypsin (a_1-AT) deficiency are relatively common single-gene disorders for which the genetic basis is known and for which current treatment strategies are not curative. On the other hand lung cancers with multifactorial nature are a complex genetic and environmental factor interaction. Attempts have been made to treat both categories by gene therapy. For any sort of gene therapy we need to develop a non-toxic, non-immunogenic, cost effective with good transformation/expression efficiency for target organ.

Here we report the development of a non-viral vector using LDL receptor mediated pathway for transporting genetic materials to the lung tissue. A tandem dimmer sequence of apoprotein-E conjugated to polylysine was used as DNA delivery vector for in vivo transformation of lung. pCDNA3.1 plasmid complexed with apoEdp-PLL harboring beta-galactosidase reporter gene was injected to the tail vein of 5 male Balb/c mices.

Frozen sections were prepared two days after injection from lung tissue and stained with X-gal for trasgene activity assay. Beta-galactosidase reporter gene activity detection kit (Sigma, USA) was used for quantitative assessment of gene expression. The beta-galactosidase activity level of 180 ng/mg of protein was detected which is indicative of acceptable transformation and activity of the transgene in the lung tissue. In all control tissues tested the values were 0.05ng/mg.

The results are very encouraging for in vivo targeted transformation using the constructed vector for gene delivery to the lung. Using specific promoter for exclusive gene expression in lung tissue virtually any gene, for cancer or monogenic diseases, could be targeted to the lung tissue.

PP-240

Metabolite profiling of *Withania somnifera* (L.) Dunal using HR-MAS NMR spectroscopy

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ABSTRACT

Withania somnifera (L.) Dunal (Solanaceae), commonly known as Ashwagandha, Indian ginseng, Winter cherry, is one of the most valued Indian medicinal plants with a number of pharmaceutical and nutraceutical applications. The extracts as well as different isolated bioactive constituents of *W. somnifera* have been reported to possess aphrodisiac, adaptogenic, anticancer, anti-convulsant, liver tonic, immunomodulatory, antioxidative and neurological effects, anti-inflammatory agent, astringent and more recently to treat bronchitis, asthma, ulcers, emaciation, insomnia, and senile dementia Gupta & Rana [1]. The major biochemical constituents of ashwaganda root and leaves are steroidal alkaloids and steroidal lactones Mishra et al. [2]. Withaferin A and withanone are the major constituents of its leaves and roots which have been reported to show a potent angiogenesis inhibitor, antitumor and anticancer activity Misra et al. [3]. Metabolic profiling of four chemotypes of *W. somnifera* was performed on fresh leaf and root tissue by HR-MAS NMR (800 MHz) spectroscopy. The HR-MAS NMR spectroscopy of lyophilized defatted leaf tissue specimens clearly distinguishes resonances of medicinally important secondary metabolites (withaferin A and withanone) and its distinctive quantitative variability among the chemotypes. A total of 41 metabolites were identified from both the leaf and root tissues of the chemotypes. The presence of methanol in leaf and root tissues of *W. somnifera* was detected by HR-MAS NMR spectroscopy. Multivariate principal component analysis (PCA) on HR-MAS ^{1}H NMR spectra of leaves revealed clear variations in primary metabolites among the chemotypes. The results of the present study demonstrated an efficient method, which can be utilized for metabolite profiling of primary and secondary metabolites in medicinally important plants.

PP-241

STUDY OF CORROSION INHIBITION PROPERTY OF HYDROXYTRIAZENES FOR COPPER IN AMMONIACAL MEDIUM

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ABSTRACT

Compound contain N,O,S have been reported to exhibit corrosion inhibitive property. Hydroxytriazene have also been reported to show efficient inhibition property for Brass in ammonical medium. In view of this the present study has been done to explore corrosion inhibition property of Hydroxytriazenes for copper metal in ammoniacal medium .Weight loss method has been used to study corrosion behaviour of copper in ammoniacal solution.

PP-242

The emerging role of chemistry in drug discovery

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ABSTRACT

The role of the drug discovery chemist has changed significantly over the past 50 years - workflows have been reinvented while the same goals remain to find and test novel molecules that can reach and act on disease targets. The role played by chemistry in the pharmaceutical industry continues to be one of the main drivers in the drug discovery process. However, the precise nature of that role is undergoing a visible change, not only because of the new synthetic methods and technologies now available to the synthetic and medicinal chemist, but also in several key areas, particularly in drug metabolism and chemical toxicology, as chemists deal with the ever more rapid turnaround of testing data that influences their day-to-day decisions.

Discovery and development of new drugs is expensive and time consuming. The estimated cost of taking a drug from discovery to market is estimated to be about US$750 million and can take between 10 and 12 years. An important question is whether a bigger investment in chemistry can make positive contributions to drug development.

Biologists initiated a revolution in the drug discovery process during the 2000s. Now it is time for the chemists to tackle the crucial issues that can be solved by chemistry, initiating a revolution by the chemists this decade. Better drugs reaching the market faster with reduced costs – that is what chemistry can and must deliver.

PP-243

A simple and efficient synthesis of some important 2-azitidinone derivatives

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ABSTRACT

A new series of Azetidinones derivatives have been synthesized from aniline derivatives in two steps.In step 1st the Schiff's bases(1a-h and 3a-h) were prepared by reacting of an aniline derivative with different aromatic aldehydes in ethanol in presence of glacial acetic acid. At 110°C(1-5).In step 2nd Cyclocondensation of the Schiff's bases(1a-h and 3a-h) with chloroacetyl chloride in the presence of triethylamine resulted in the formation of the corresponding Azetidinones compounds(2a-h and 4a-h):The structures of the newly synthesized compounds (2a-h and 4a-h) are confirmed by IR, 1H NMR spectroscopic analysis (6-8).

PP-244

Role of some metal ions in photocatalytic bleaching of 'rose bengal' dye

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ABSTRACT

The photocatalytic bleaching of Rose Bengal was carried out in the presence of semiconducting zinc oxide and was observed photocolourimetrically. The effects of various operating variables like pH, concentration of dye, amount of semiconductor and light intensity on the efficiency of the reaction were also observed. Attempts have been made to study the effect of the addition of other metal ions like Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+} $Cu^{2+}$and Zn^{2+}. Some of the added metal ion like Fe^{2+}, Co^{2+} and Cu^{2+} increase the reaction rate to some extent while Mn^{2+}, $Ni^{2+}$and Zn^{2+} decrease the reaction rate to some extent. It is also observed that Cu^{2+} is most effective in bleaching of Rose Bengal. A tentative mechanism has been proposed.

PP-245

Molecular characterization of an evolutionary conserved principle of plant defense

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ABSTRACT

In this report we have characterized a unique interaction between certain type I ribosome-inactivating proteins (saporin) and triterpenoid saponins. Both components are biosynthesized by the plant *Saponaria officinalis* L. Here we show that triterpenoidsaponins specifically mediate the release of saporin out of the intracellular compartments into the cytosol without affecting the integrity of the plasma membrane. The relevant cellular compartments were identified as late endosomes and lysosomes. Further studies revealed that endosomal acidification is a prerequisite for the saponin-mediated release of saporin. Binding analysis demonstrated an association of the saponins with saporin in a pH-dependent manner. The applicability of the saponin-mediated effect was demonstrated *in vivo* in a syngeneic tumor model using a saporin-based targeted anti-tumor toxin in combination with characterized saponins.

PP-246

Heliotropium Indicum seeds as corrosion monitor

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ABSTRACT

A large number of chemicals are used for corrosion inhibition without much knowledge of their toxicity environmental impact.So today's needs is to produce and use better green product with less waste and without damaging the earth's eco-system.In continuation of this we have used a weed (*Heliotropium Indicum*-family Boraginaceae) which is easily available and accessible.The corrosion inhibition of Al by alcoholic extract of seeds from *Heliotropium Indicum* has been studied using mass loss method.It was found that the different concentrations of alcoholic extract of *Heliotropium Indicum* inhibit Al corrosion.It is concluded that the inhibition efficiency increased with the increase in concentration of inhibitor.The entire study shows that the seed extract of the *Heliotropium Indicum* is a non-toxic,cost effective corrosion inhibitor for Al in acidic medium.

PP-247

Novel water soluble *N*-mustard-benzene conjugates with potent antitumor activity, synthesis and biological activity

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ABSTRACT

The solubility of compound is one of the important factors for determining the success of the agent during drug development. We have previously reported a series of water-soluble N-mustards-benzamide conjugates having hydrophilic side-chain at the *meta*- or *para*-position of the carboxamide group via a urea spacer. Of these derivatives, BO-1055 HCl exhibits a broad spectrum of antitumor activity and potent therapeutic efficacy against various human solid tumor xenografts. Recently, we have synthesized a series of novel water soluble *N*-mustard-benzene conjugates prepared by linking phenyl *N*-mustard pharmacophore with benzene moiety through urea linker. The benzene ring bears a variety of ?-*N*,*N*-dialkylaminoalkylamide or ?-cyclicaminoalkylamide side-chains located to the *meta*- or *para*-position of the urea linker. The tertiary amino function on the side-chain can be converted into a variety of water-soluble salts with various acids. The newly synthesized derivatives were subject to evaluate their antitumor activities both in vitro and in tumor xenograft model. The results showed that these conjugates exhibit a broad spectrum of antitumor activity against variety of human leukemia and solid tumor cell growth in culture. Among these derivatives, **BO-2094** was selected for further antitumor evaluation. The results revealed that this agent exhibited potent antitumor activity several human tumor xenografts in animal model. Studies on the mechanism of action revealed that **BO-2094** is able to induce DNA cross-linking and arrest cell cycle at G2/M phase. The present studies suggest that **BO-2094** is a promising candidate for preclinical antitumor studies.

PP-248

Microwave assisted solvent free synthesis of substituted phenyl-1-(2, 4-dinitrophenyl)-4, 5-dihydro-1H-pyrazolo (3, 4-d) pyrimidine 3,6(2H,3aH)-dione derivatives in ionic liquid

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ABSTRACT

Microwave induced organic reaction enhancement has been described by Bose et al [1]. as a safe and convenient alternative to pressure reaction in unmodified microwave ovens with several advantages of an eco-friendly approach. In the present work synthesis of an ionic liquid containing imidazolium moiety has been reported by a novel method. The synthesized ionic liquid has been characterized by IR, NMR and mass spectral data. Using the synthesized ionic liquid as a reaction medium synthesis of substituted phenyl-1-(2, 4-dinitrophenyl)-4, 5-dihydro-1H-pyrazolo (3, 4-d) pyrimidine 3, 6(2H, 3aH)-dione derivatives have been carried out under microwave irradiation. The synthesized compounds have been characterized by different spectral techniques i.e. IR, ^{1}H NMR and Mass spectra.

PP-249

6-Gingerol improves 2-^{3}H-Glucose uptake in cultured L6 cells by regulating the mitochondrial biogenesis

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ABSTRACT

The rhizomes of *Z. officinale* is commonly known as ginger which has been widely used as a spice in our food. The medicinal properties of rhizome of Z.officinale are well documented in Ayurvedic, Chinese and Tibb-Unani systems of herbal medicine. Various oleoresins isolated from rhizhomes of ginger including gingerol, shoagol, and zingerone, have been found to possess many pharmacological and physiological activities. Earlier report from our laboratory shows that gingerol possess both anti-

hyperglycaemic and antidyslipidemic properties (Singh et al (2009) International J. Med. Sci., 1(12), 536-544) (1). To further evaluate the role of 6-Gingerol in control of glucose homeostasis we studied the 2-^{3}H-glucose uptake by muscle myotubes treated with 6-Gingerol and performed gene expression studies. Results indicates that 6-Gingerol increases the glucose uptake in muscle myotubes (L6) in a dose dependent fashion and gene expression analysis reveals that expression of PPAR? Coactivator 1 alpha (PGC 1a), NRF-1, GLUT4 , Cox 1, Cyt c, Citrate synthase and mtTFA increased in myotubes treated for 16 hours with 6-Gingerol. Increase in expression of PGC 1a confirms the increase in mitochondrial biogenesis in response to treatment of L6 myotubes with 6-Gingerol which is further confirmed by increase in expression of mitochondrial markers Cox 1, Cyt c and Citrate synthase. Over expression of NRF-1 resulted in increased expression of myocyte enhancer factor (MEF) 2A and the GLUT4 isoform of the glucose transporter in muscle(2) this confirms the improvement of glucose uptake in muscle myotubes on treatment with 6-Gingerol. Functional NRF-1 and NRF-2 binding sites have been identified in the promoter of the nuclear gene that encodes mtTFA, a transcription factor that regulates mitochondrial DNA transcription and replication. This studies shows the possible role of 6-Gingerol in improvement of glucose metabolism in cultured L6 myotubes by increasing the mitochondrial biogenesis.

PP-250

Synthesis and In-silico activity prediction of some schiff bases of p-aminoacetophenone containing hydroxytriazene moiety

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ABSTRACT

In a search for new leads potent chemotherapeutic agents are being attempted in recent years. In the present study, an array of Schiff bases containing hydroxytriazene [1] moiety (i-v) have been synthesized and characterized through their spectral and physical analysis. For this, p-aminoacetophenone and isoniazide were condensed in methanol media to yield Schiff base [2]. Amino group of the resulting Schiff base was diazotized and coupled with various phenylhydroxylamines obtained by reduction of corresponding nitro compounds to give title compounds (i-v). The PASS (Prediction of Activity Spectra for Substance)[3] for compounds has been done which indicates potent antitubercular, antimycobacterial, antineoplastic, anemia sidroblastic, and antibacterial activities. The present study, thus paves a way for Computer Aided Drug Designing (CADD).

PP-251

Microwave assisted synthesis of some spiro-[indole-thiazolidine] derivatives: a green chemical pathway

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ABSTRACT

Heterocyclic compounds hold a special place among pharmaceutically important natural and synthetic materials. The remarkable ability of heterocyclic nuclei to serve as reactive pharmacophores, has largely contributed to their unique value as traditional key element of numerous drugs. Spiro compounds are well known to posses varied pharmacological activities [1,2] The reaction sequence involves microwave induced preparation of N-(2-oxo-1,2-dihydro-3'H-indol-3-ylidene)pyridine-4-carbohydrazide from isoniazid and isatin followed by the cyclocondensation of N-(2-oxo-1,2-dihydro-3'H-indol-3-ylidene)pyridine-4-carbohydrazide and mercaptoacetic acid under microwave irradiations to achieve the synthesis of spiro-[indole-thiazolidine] compound. The resulting compound was then allowed to react with various aromatic aldehydes to afford arylidene derivatives.

PP-252

STUDIES ON THE ELECTROCHEMICAL BEHAVIOR OF LANTHANUM COMPLEXES OF HYDROXYTRIAZENES

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ABSTRACT

Lanthanum (III) complexes of hydroxy triazene have been studied in our laboratory earlier. In the present study are attempt has been made to study La(III)-3-hydroxy-3-p-tolyl-1-p-sulphonamidophenyltriazene (HPST) complex by polarographic method. The study has been done in Britton-Robinson (B-R) buffer at constant ionic strength of KCl (0.01N). Lingane method has been used to determine stability constant and log ß has been found to be 26.9. This is first polarographic method report for 3-hydroxy-3-p-tolyl-1-p-sulphonamidophenyltriazene (HPST) -La (III) complexes.

PP-253

Synthesis, Characterization and Antimicrobial Evaluation of Some 6-substituted-3-chlorobenzo[b]thiophene Derivatives

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ABSTRACT

In the present investigation, a series of 3-chlorobenzo[b]thiophene[1] derivatives of N'-(3-(3-chlorobenzo [b]thiophene-2-carbonyl)-4-oxothiazolidine-2-ylidene)-7-methyl-3-oxo-5-phenyl-3,5-dihydro-2H-oxazolo [3,2-a] pyrimidine-6-carbohydrazide **5a-d** and 3-chloro-N-(5-(7-methyl-3-oxo-5-phenyl-3,5-dihydro-2H-oxazolo[3,2-a]pyrimidine-6-yl)-1,3,4-thiadiazole-2-yl)benzo[b] thiophene -2-carboxamide **8a-d** have been synthesized starting from ethyl-6-methyl-2-oxo-4phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate **1** via a multistep reaction sequence. The structure of all synthesized compounds has been confirmed by different spectral studies. Final compounds have been screened for their antimicrobial activity.

PP-254

FLOURIDE POISON THROUGH DRINKING WATER IN POPOLACE OF DEOLI AREA OF TONK DISTRICT (RAJASTHAN) AND HEALTH HAZARDS

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ABSTRACT

Drinking water is a major source of flouride uptake that causes flourosis. According to World Health Organisation WHO, 1996 [1] guidelines flouride concentration should remain below 1 ppm. However, this value for Indian climate WHO standards and BIS, 1991 [2] permit only 1.5 ppm as a safe limit. In fact, Flouride is beneficial in prevention of cavities formation in the teeth and provide strength to skeleton system. However, long term consumption of water containing excessive amount of flouride causes flourosis that affects teeth, bones, joints and ultimately leads to crippling. Flourosis is not common only in India but many countries like USA, China, Japan, Argentina, African and Gulf countries, etc are affected even more Webber, J.T., 2009 [3]. Rajasthan state is thought to be the most seriously affected by high flouride, all 33 district are endemic for flourosis. Flouride concentrations in groundwater of Deoli Area varied from 0.70 ppm to 9.0 ppm. Populace of this area suffering from dental as well as skeletal Flourosis. The Nalgonda technique is suggested due to an economical way for deflouridation.

PP-255

Azaspirocycles in Small Molecule Drugs: A Molecular Docking Investigation

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ABSTRACT

Azaspirocycles are spirocyclic compounds containing at least one N. These structures can be regarded as interesting surrogates for piperazines, piperidines, morpholines and and thiomorpholines which are present in several marketed drugs.[1] There are some inherent metabolic or toxicological liabilities associated with piperazine (N-oxide formation), morpholine (oxidative degradation) and piperazine (hERG inhibition). Replacing piperazine by spiropiperazine, morpholine by spiromorpholine and piperidine by spiropiperidine may lead to improvement in physicochemical and/or pharmacokinetic properties. The present investigation details the effects of replacing these substructures by their spirocyclic counterparts in crystal structure ligands of therapeutically relevant drug targets using molecular docking. The effects of these structural changes on physicochemical and/or pharmacokinetic properties are also studied. The replacement by azaspirocycles may result into structurally novel molecules. It can be regarded as a viable strategy in the medicinal chemistry of small molecule drugs containing piperazine, morpholine and piperidine.

PP-256

KINETICS AND CORRELATION ANALYSIS OF REACTIVITY IN THE OXIDATION OF SUBSTITUTED BENZALDEHYDES BY BENZIMIDAZOLIUM DICHROMATE

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ABSTRACT

Kinetic and mechanistic studies of the oxidation of a number of *para*-, *meta*- and *ortho*-substituted benzaldehydes by benzimidazolium dichromate (BIDC), in dimethyl sulphoxide, were discussed with an emphasis of correlation of structure and reactivity. The product of the oxidation is the corresponding benzoic acid. The reaction is first order with respect to BIDC, however, the dependence is of second order with respect to hydrogen-ion. Michaelis-Menten type kinetics were observed with respect to aldehyde. The deuterium isotope effect for the oxidation of [^{2}H] benzaldehyde (k_H/k_D = 6.17 at 293 K) indicated an a-C-H bond cleavage in the rate-determining step. Based on kinetic data, analyses of the solvent effect and results of structure-reactivity correlation along with some non-kinetic parameters suggested a mechanism involving rate-determining oxidative decomposition of an aldehyde-BIDC complex *via.* a cyclic transition state to give a carbocationic species through hydride-ion transfer from the aldehyde to the oxidant.

PP-257

Ecofriendly Microwave Assisted Synthesis of Pyrazole derivatives and their Biological behavior

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ABSTRACT

The utilization of green chemistry technique is dramatically reducing chemical waste and reaction time has been proven in several organic synthesis and chemical transformation. Microwave-assisted organic synthesis is an enabling technology for accelerating drug discovery and development processes. Pyrazole are well known and important five membered heterocyclic compounds and various methods have been worked out for their synthesis.[1-2] Therefore, in this work a new series of pyrazole derivatives have been synthesized by different chalcones under microwave irradiation. These derivatives have been screened for their antimicrobial activity against different microorganism. Mosquito larvicidal activity of the synthesized compounds is also have been studied. The structures of synthesized compounds have been established on the basis of elemental analysis IR, ^{1}HNMR and mass spectral data.

PP-258

Synthesis and characterization of some conducting polyanilines

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ABSTRACT

Polyaniline (PANI) is a polyaromatic amine that can be easily synthesized chemically from bronsted acid aqueous solutions containing aniline. It is one of the best and potentially useful conducting polymer and has received considerable attention in recent years because of its environmental stability, low cost of raw material and easy synthesis [1]. These materials for being polyconjugated systems having alternate simple and double bonds, possess a considerable electron availability, which provide them with a rigid structure and a better capacity to be adsorbed on metallic surfaces [2]. PANI found a wide variety of applications in polymeric batteries, smart windows, membranes, anticorrosion coatings, sensor devices, high conductivity and environmental stability [3]. The common chemical synthesis of PANI is a stoichiometric route and utilizes harsh reagents such as a strong oxidant and strong mineral acid [4]. The most widely used route to polyaniline involve $(NH4)_2S_2O_8$ as oxidant which generates significant amount of $(NH4)_2SO_4$ as by product. In the present work, polyanilines have been synthesized using different types acidic conditions. The structure of polyanilines were elucidated by UV- vis, FTIR and NMR spectroscopy which confirmed the presence of benzenoid and quinoid rings in the polyanilines. Molecular weight has been determined by GPC analysis. TGA results and conductivity studies showed that samples had good thermal stability and electroactivity.

PP-259

Analytical application of 2, 2'-[piperazine-1,4-diyl-diazene-2,1-diyl]bis(1,3benzothiazole) in the spectrophotometric determination of Iron (III) and its fluorescence applications

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ABSTRACT

Triazenes are a unique class of polyazo compounds containing 3 consecutive N atoms in an acyclic arrangement[1-3]. In the present work, a new triazene viz., 2, 2'-[piperazine-1,4-diyl-diazene-2,1-diyl]bis(1,3-benzothiazole) (PDBB) has been synthesized by the reaction of piperazine with 2 equivalent of the appropriate diazonium salt, yielding orange–red coloured product. The compound was duly characterized using IR, Melting point determination, and other physicochemical techniques. PDBB has been used for spectrophotometric determination[4-5] of iron (III) at 530 nm and at pH range of 2.5-4.0. The compound also shows fluorescence properties as evidenced by its emission spectra at 350 nm and 415 nm. Thus, the present studies have brought about an excellent spectrophotometric reagent showing fluorescent properties. It can be further explored as a molecular sensor.

PP-260

Enhancement of Bioavailability of Exemestane “A breast cancer drug” by Cyclodextrin Complexation

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ABSTRACT

Exemestane (EXE) is a third generation irreversible aromatase inhibitor, approved by FDA to be used for advanced breast cancer in post menopausal women. It is an orally administered class IV drug with a bioavailability of only 5%, having low solubility and extensive first pass metabolism. Therefore, in order to improve its solubility and hence bioavailability, an approach has been made towards development of its cyclodextrin (CD) complexation uing various cyclodextins. The solubility of cyclodextrins was found to be Methyl-Beta-CD (methyl – ß –CD) > Gamma-CD (?-CD) > Beta-CD (ß-CD) > Alpha-CD (a-CD). As per the study, methyl-ß -CD was found to be a good candidate, but it was not used because of its oral toxicity. So the second best CD i.e ?-CD was selected as it has no oral toxicity and has been approved by USFDA (United States Food and

Drug Administration) as GRAS (Generally Recognized as safe). Phase solubility studies were performed with ?-CD. Based on AL- type curve, 1:1 molar ratio of EXE: ?-CD was selected for preparation of freeze dried complex. Solid state characterization of the complex was carried out by DSC, FTIR, NMR, XRD and SEM. Dissolution studies were conducted and a significant improvement in the dissolution profiles of the aromatase inhibitor prepared as inclusion complex was observed A sensitive, specific and rapid analytical method for the quantification of EXE in human plasma was developed using HPLC. The method was fully validated in the concentration range of 50-5000 ng. Oral pharmacokinetic study was performed in female wistar rats (n=6) divided into two groups at a dose of 25 mg/70 kg body weight. In conclusion, EXE complexation with cyclodextrins results in an enhancement of solubility, and hence an increased bioavailability of the drug.

PP-261

Potential Hyper-mutable Repetitive Sequences In Flanking Sequences of Human Genes

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ABSTRACT

Repetitive sequences are hyper-mutable DNA sequences containing mono to hexa nucleotide repeat units repeated in tandem. Instabilities in these repeats are known causes of many disorders. The present study was undertaken to explore tandem repeats in flanking sequences (FS) of human genes with specific reference to replication and repair genes and compared with mammalian orthologues. The present study shows higher number of tandem repeats in upstream FS in genes of some mammals whereas; in others these repeats are higher in downstream FS. This paper presents *in silico* analysis and characteristics of tandem repeats occurring in FS of human genes and their conservation in mammalian orthologues. These repeats may be potential mutational hotspots that could be used for further exploration of their potential roles in gene regulation or medical investigations.

PP-262

Copper Vanadium Oxide as heterogeneous photo-Fenton like catalyst for the degradation of Neutral red

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ABSTRACT

Different processes have been developed to treat waste water from textile industries such as filtration, biological adsorption process, electrochemical process, oxidation by ozone etc. But all of these processes suffer from one or more drawbacks related to cost, time or sludge formation etc. however, in last few years much attention has been paid on the development of Advanced Oxidation Processes (AOP's) for the treatment of waste water and effluents from various industries. Mosteo et al. [1] reported the photo-Fenton process in heterogeneous phase as an advanced oxidation methodology for the treatment of winery waste water. Zhang et al. [2] suggested application of heterogeneous catalyst of tris (1, 10)- phenanthroline iron (II) loaded on zeolite for the photo-Fenton degradation of methylene blue. In the present work, degradation of neutral red under visible light has been investigated using copper vanadium oxide as heterogeneous photo-Fenton like catalyst, which has been prepared by wet chemical method. The synthesized photocatalyst has been characterized by XRD, SEM, EDS, FT-IR, TGA/DSC and BET. The effect of variation of different parameters i.e., pH, amount of photocatalyst, concentration of dye, amount of H_2O_2, light intensity has been observed on the rate of reaction. The rate of photocatalytic degradation of dye follows pseudo first order kinetics.

PP-263

Bis-Hydroxytriazenes: A new class of analytical reagent

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ABSTRACT

A simple, rapid and sensitive spectrophotometric method has been developed for the determination of Iron (III) using 4, 4'sulfonyl bis(phenyl-3-(4-methylphenyl)-3-hydroxytriazene). The proposed method is based on the diazotization of Dapsone [1-2] followed by coupling with 4methylphenylhydroxylamine [3] in alkaline medium to give intense yellow coloured product duly characterized by spectral and physical analysis. Title compound gave green colour with Fe(III). 4, 4'sulfonyl bis(phenyl-3-(4-methylphenyl)-3-hydroxytriazene) has been used for spectrophotometric determination [4] of iron (III) at 570 nm and at pH range of 3.0-4.5.

PP-264

Spectrophotometric Determination of Zinc (ll) With Hydroxytriazenes and Schiff's Base

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ABSTRACT

A number ofhydroxytriazenes along with Schiff's base were considered to be suitable for their use as Spectrophotometric reagents for quantitative determination of Zinc (ll) by mixed ligand technique. The spectrum of acetonic solution of each complex of Zinc (ll) with each of the hydroxytriazenes and Schiff's base were recorded in wavelength region of 380-500 nm under optimum p^Hconditions. For this purpose Zinc (ll), one of the hydroxytriazenes and Schiff's base were taken in molar ratio of 1:10:10 and p^H was so adjusted that colour intensity was visibly maximum. It has been observed that ternary complex in each case has higher absorbance as compared to the binary complexes, in view of this wavelength of maximum absorbance ($?_{max}$) of ternary complex was used as working wavelength. The composition of the temary complex of Zinc (ll) with Schiff's base and each of the hydroxytriazenes was determined spectrophotometrically by Yoe and Jones mole ratio method. From the pair of mole-ratio curve for each ternary complex, it has been concluded that composition of each ternary complex was-Zn:hydroxytriazenes: Schiff's base:: 1:1:1.The molar absorptivity values of ternary complexes of Zinc (ll) with each of the hydroxytriazenes and Schiff's base have been determined from the corresponding Beer's Law curve. Using these values of molar absorptivity, Sandell's spectrophotometric sensitivity values have been calculated.

PP-265

Synthesis of some novel benzothiazines and ribofuranosides as possible Antimircobial agents

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ABSTRACT

BenzothiazinesVI,10H-acetyl-8-chloro-7-fluoro/6-chloro-9-methyl/9-ethyl-3-nitro-pyrido [3,2-Zb] [1,4] benzothiazines VII and 10H-8-chloro-7-fluoro/6-chloro-9-methyl/9-ethyl-3-nitro-pyrido[3,2-b][1,4]benzothiazine-5-oxides VIII have been synthesized. *?* -D-ribofuranose-1-acetate-2,3,5-tribenzoate on refluxing with compound VI affords N-(2′,3′,5′-O-benzoyl-*?* -D-ribofuranosyl)-8-chloro-7-fluoro/6-chloro-9-methyl/9-ethyl-3-nitro-pyrido[3,2-b][1,4]benzothiazines IX.
Structural assignments of these compounds have been made on the basis of elemental analysis like IR, ^{1}H-NMR [1] and these compounds have also been screened for their antimicrobial activities and characteristics.

PP-266

An ICT based fluorescent pH sensor for bioimaging.

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ABSTRACT
Small molecule fluorophores those undergo drastic change in photo physical property through PET or ICT process upon interaction with the analyte are emerging as popular tools for detection of analytes in biological substances [1]. There are two types of fluorescent probe for cellular pH imaging, one is for cytosol which generally remains near neutral pH another is for the acidic organelles which generally remain near pH 5.5-3.5 [2]. Fair number of fluorescent molecular probes working near neutral pH has been reported till date but florescent molecular probes for acidic organelles are still rare. In this work we have investigated 2-phenyl hydrazinylidene)methyl]quinoline (PHQ) as a new charge transfer pH fluorescent and chromogenic probe for bio imaging of acidic organelles. The acidic and basic forms of the probe are characterized by NMR, FTIR, and single crystal X-ray diffractometry. The presence of Na^+, K^+, Ca^{2}+, Mg^{2+} and transition metal ions does not interfere with its fluorescent pH response. In addition, the intracellular pH fluorescent imaging ability of the probe has been confirmed on Hela cells using a fluorescence microscope.

PP-267

Conservation Genetics of endangered medicinal plant *Commiphora wightii* in Indian Thar Desert

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ABSTRACT
To ascertain the conservation priorities and strategies for *Commiphora wightii*, an endangered medicinal plant of Indian Thar Desert, genetic diversity was estimated within and among different populations. The total of 155 amplification products were scored using ten each of RAPD and ISSR primers, exhibiting an overall 86.72% polymorphism across 45 individuals representing eight populations. The cumulative data of two markers were used to compute pair-wise distances. The NJ tree after a 1000 replicate bootstrap test of robustness revealed high genetic differentiation among populations except Kiradu population. Nei's gene diversity (h) ranged between 0.082-0.193 with total diversity at species level is 0.294. Shannon's information index (I) ranged between 0.118-0.275 with an overall diversity of 0.439. Analysis of molecular variance showed more diversity among population (56.65%) than at within population level (43.35%). The low gene flow value (Nm = 0.349) and high coefficient of genetic differentiation (G_{ST} = 0.589) and high fixation index (F_{ST} = 0.566) demonstrated elevated genetic differentiation among the population and can be predicted that these populations are not in Hardy–Weinberg proportions. Principle Coordinate Analysis confirms that Akal population has become phylogenetically more distinct and less diverse than rest of the samples. Mantel's test revealed no correlation between genetic and geographical distances of populations (R^2 = 0.122). Overall high diversity was observed in the population of Machiya Safari Park and Kiradu, while low in Akal population, later may constitute evolutionary significant unit, having merit for special management.

PP-268

Analysis of physico chemical characteristics of water of Ayad River at Udaipur, Rajasthan

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ABSTRACT
The present study was conducted to evaluate water pollution status of Ayad River after crossing the urban and industrial area of Udaipur. Ayad River is very old river which passes through the heart of Udaipur city, it carries waste water containing urban and industrial effluents. Two sampling stations were identified where sampling station A represents domestic effluent station and sampling station B represents industrial effluent station. The water quality variables were analyzed as per standard methods given in American Public Health Association (APHA, 1989). Water quality parameters such as pH, temperature, conductivity, TDS, DO, BOD_5, COD, TOC, acidity, alkalinity, total hardness, chloride, nitrate, phosphate, MPN, and heavy metals were analyzed and results were compared with the control water sample which was distilled water..

PP-269

Electronic Structure of Explosive Materials using Compton Scattering Study

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ABSTRACT

In this paper, we report the Compton profile studies of energetic materials namely KNO_3 and NH_4NO_3 using linear combination of atomic orbitals (LCAO) within density functional theory (DFT) and its hybridization with Hartree-Fock (HF). The theoretical Compton profiles are compared, for the first time, with the experimental profiles measured using 100 mCi ^{241}Am Compton spectrometer (in case of KNO_3) and 20 Ci ^{137}Cs Compton spectrometer (for NH_4NO_3). It is seen that the hybrid functional involving HF and DFT approximations gives a relatively better agreement with experimental momentum densities than other approximations of DFT. The bonding of valence electrons is explained in terms of localization of their wave functions and the charge densities.

PP-270

Synthesis and DNA Cleavage Studies of Trinuclear Cu(II) Complexes

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ABSTRACT

DNA binding is the main biological event that triggers the anticancer properties of the metal complexes. Studies on the interaction between the transition metal complexes and DNA are important to further understand their pharmacology.

Copper is third most abundant transition metal ion in the biological system, and it controls several electron transfer and oxidative processes. Recently, the structure of a number of mono [1,2], di [3-4], tri [1,2,5,6] and tetra [5] nuclear copper complexes derived from glycosylamine based Schiff's base has been established, however their applications are yet to be explored. Coordinatively labile trinuclear Cu(II) complex derived from glycosylamine based ligand has been used in proton transfer reaction [5] and C–Cl bond activation of solvent chloroform at room temperature [1,2]. Dinuclear Cu(II) complexes derived from similar ligands have been used in selective oxidation of primary and secondary alcohols into corresponding carbonyl compounds [6] and DNA cleavage studies [4]. Recently we have explored the DNA cleavage activities of sugar containing trinuclear Cu(II) complexes and the same will be presented in the conference.

PP-271

Electronic properties of 10% Co doped ZnO dilute magnetic semiconductor

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ABSTRACT

In this paper, we present preparation of a dilute magnetic semiconductor (DMS) namely 10% Co doped ZnO using solid state reaction method. To measure the Compton profile, we have used our 20Ci Cs^{137} Compton spectrometer at an intermediate resolution. The theoretical Compton profiles, band structures and density of states of the DMS were also calculated using linear combination of atomic orbitals (LCAO) within density functional theory (DFT). It is found that the experimental and theoretical Compton profiles reconcile well in the high momentum side. Differences in the low momentum region are attributed to the quality of basis sets. The charge density is also discussed in base material ZnO and the doped compounds to discuss the effect of bonding on the doping.

PP-272

Photocatalytic Degradation of Bromocresol Green by Well-Dawson Heteropoly Anion in Aqueous Medium

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ABSTRACT

Potable water is a main need of everyone including human being, animal and plant kingdom. Effluents of different textile, dyeing and printing industries, which are being discharged in nearby water resources, are creating water pollution. Use of a semiconductor as photocatalyst is considered as a promising technology, which provides solution for this problem. In the present investigation, the photochemical degradation of Bromocresol green by Well-Dawson heteropoly anion has been carried out. The rate of photocatalytic degradation of dye was observed spectrophotometrically. The effect of different parameters, which affect the rate of reaction; like pH, concentration of dye, amount of semiconductor and light intensity has been studied for the above system. Kinetic studies reveal that the photocatalytic process follows pseudo-first order kinetics. A tentative mechanism for the photocatalytic degradation of Bromocresol green has also been proposed.

PP-273

Synthesis of Pharmacologically active 6,8-Dimethyl 4*H*-1,4-benzothiazines and their sulfones

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ABSTRACT

Heterocyclic compounds are highly ranked among the pharmaceutically important natural and synthetic materials. The remarkable ability of heterocyclic nuclei to serve as both biomimetics and pharmacophores has largely contributed to their unique value as traditional key elements of numerous drugs. Heterocycles containing N & S i.e. 4H-1,4-benzothiazines are found active as sedative, antispasmodic, antiulcer, bactericide, antioxidant and anticancer agents. 4*H*-1,4-benzothiazines were prepared by condensation followed by oxidative cyclization of 2-amino-4,6-dimethylbenzenethiol with β-diketones / β-ketoesters in DMSO. On refluxing with hydrogen peroxide in glacial acetic acid, these substituted 4H-1,4-benzothiazines yielded 4H-1,4-benzothiazine-1,1-dioxides (sulfones). The structure of the synthesized compounds have been confirmed by spectral and elemental analysis. These compounds were evaluated for antimicrobial and antioxidant activities.

PP-274

Magnetisation in 5% Ni doped $La_{0.7}Ca_{0.3}MnO_3$

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ABSTRACT

In this paper, spin-polarized electron momentum distribution of Ni doped $La_{0.7}Ca_{0.3}MnO_3$ manganite at 250K temperature has been measured using magnetic Compton spectrometer at SPring-8, Japan [1]. It is seen that the spin moment reduces from 2.65 μ_B/f.u. to 0.39 μ_B/f.u. on doping of Ni at Mn site. To visualize the role of Mn in doped and undpoed compound, the magnetic profile is splitted into constituent profiles. It is seen that the diffuse contribution is coupled antiferromagnetically to spin moment arising from 3d electrons of Ni and Mn.

PP-275

Electronic properties of rare earth dioxide CeO_2

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ABSTRACT

In this paper, we present electron momentum densities of CeO_2 using 20 Ci ^{137}Cs Compton spectrometer [1]. To extract the true Compton line shape, the raw data have been corrected for several systematic corrections like background, tail stripping, Compton cross-section, multiple scattering, etc. To compare our experimental data, we have also computed theoretical Compton profiles using linear combination of atomic orbitals (LCAO) within the frame work of density functional theory (DFT). We have also calculated the Mulliken's population, energy bands and density of states using the LCAO method. The energy bands and density of states obtained from the present calculations show insulator character of CeO_2. The role of 4f electrons is discussed in the formation of electronic structure of the compound. The experimental Compton profile shows a better agreement with generalized gradient approximation within the DFT.

PP-276

Laboratory Evalutaion on the Potential of Entomopathogenic Fungi Beauveria Bassiana (Balsamo) Vuillemin (DEUTEROMYCOTINA: HYPHOMYCETES) Against Termite Funa of SOUTH RAJASTHAN

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ABSTRACT

Termites are exopterygotous, social insects which belong to the order Isoptera that build nests in the soil or wood. Their presence is particularly noticeable in tropical and subtropical regions where they represent a significant portion (10%) of the animal biomass.At the same time some species cause extensive damage to agriculture crops such as maize, wheat, vegetables, sugarcane etc., forest, stored food, woodworks in building in India and many other countries of the world, since the principle food is cellulose. The economic losses associated with termite damage for India 35 million US dollars. Development and application of formulations of the microbial could supplement existing termite control methods and reduce dependence on synthetic chemicals. *Beauveria bassiana* (Balsamo) is one of the several natural biocontrol agents for controlling the termite by direct penetration of the insect cuticle. Therefore, the purpose of this study was to determine the pathogenicity by *Beauveria bassiana* (Balsamo) on termite workers as this caste only is the most destructive caste. Four different conc. 4.5×10^5, 4.5×10^6, 4.5×10^7 and 4.5×10^8 conidia/ ml of conidial suspension of *Beauveria bassiana* (Balsamo) were applied on filter paper disc. After twenty four hours of inoculation, the workers were found with progressive symptoms of sluggishness (slow movement) and weakness. Presence of melanized spots on the cuticle near the thoracic and abdominal segments of worker termites were quiet prominent. Mortality observed after 72 hours of post inoculation of highest dose (4.5×10^8 conidia/ ml)was 95% as compared to 18% in control at same period. After seven days the white mycelia of fungus developed on cadavers. Fungal colonies were also clearly visible throughout the ventral portion of the body, which suggest that fungal growth can cause serious damage to the pest disturbing its major physiological activities resulting in its death. Hence, this study cleared revealed that *Beauveria bassiana* (Balsamo) can be considered as an efficient tool for the control of termite in laboratory conditions and has the potential to be developed as a microbial biopesticide for controlling the termite colony.

PP-277

INTERACTION OF ANTIBACTERIAL DRUG AMPICILLIN WITH GLYCINE AND ITS DIPEPTIDES ANALYZED BY VOLUMETRIC AND ACOUSTIC METHODS AT DIFFERENT TEMPERATURES

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ABSTRACT

The interactions of glycine (gly), glycylglycine (gly-gly), glycylleucine (gly-leu) with drug ampicillin as a function of temperature have been investigated by combination of volumetric and acoustic methods. Densities and speeds of sound of glycine and its dipeptides in aqueous solutions of ampicillin have been measured at T = (305.15, 310.15 and 315.15) K and atmospheric pressure. The apparent molar volume ($V_?$), the partial molar volume ($V_?^0$) and standard partial molar volumes of transfer ($?V_?°$) for glycine and its dipeptides from water to aqueous ampicillin solutions have been calculated from density data. Partial molar adiabatic compressibility ($K_?$) and partial molar adiabatic compressibility of transfer ($?K_?^0$) have been calculated from speed of sound data. The pair and triplet interaction coefficient have been calculated from both the properties. The absorption spectra have also been recorded for present mixtures with the help of UV-visible spectrophotometer. The results have been explained on the basis of competing patterns of interactions of co-solvents and the solute.

PP-278

Insight into the role of *Mycobacterium tuberculosis H37Rv* MoaC2 in molybdenum cofactor biosynthesis based on the structural characterization

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ABSTRACT

The Molybdenum cofactor (Moco) biosynthesis pathway is an evolutionary conserved pathway seen in almost all eukaryotes including the pathogenic species *Mycobacterium tuberculosis* H37Rv. This pathway comprises of several novel reactions, which include the initial formation of precursor Z from guanosine triphosphate (GTP), which is catalyzed by MoaA and MoaC enzymes [1]. Although Moco biosynthesis is well understood, the first step is still not clear. In *M. tuberculosis H37Rv*, three orthologous genes of MoaC have been annotated: moaC1 (Rv3111), moaC2 (Rv0864) and moaC3 (Rv3324c). Rv0864 (MoaC2) is a 17.5 kDa protein and is reported to be down-regulated by ~3 times in the nutrient starvation model for *Mycobacterium tuberculosis* [2]. Full-length MoaC2 (17.5 kDa, 167 residues) was cloned in Escherichia coli and purified to homogeneity. Crystals of recombinant M. tuberculosis MoaC2 were grown by vapour diffusion using a hanging-drop setup. The crystal belonged to the cubic space group P2(1)3, with unit-cell parameter 94.5 Å. Matthews coefficient (V(M)) calculations suggested the presence of two molecules in the asymmetric unit, corresponding to a solvent content of about 39%. Molecular-replacement calculations using the E. coli homologue as the search model gave an unambiguous solution. The crystal structure of Moco-biosynthesis protein MoaC2 from *Mycobacterium tuberculosis* (2.20 Å resolution) has been determined. The functional roles and the residues involved in oligomerization of the protein molecules have been identi?ed based on a comparative analysis of structure with those of homologous proteins. Molecular docking studies were carried out in order to identify its ligand. Sequence based interaction study identified MoaA1 to interact with MoaC2. A homology model of MoaA1 was then complexed with MoaC2 and protein–protein interactions are also discussed.

PP-279
Studies on *in vitro* regeneration in groundnut and characterization using biochemical and histological studies

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ABSTRACT

In living cells reactive oxygen species (ROS) are an inevitable product of aerobic respiration and stress conditions. *In vitro* plant cultures are subjected to stress conditions resulting in ROS production. ROS functions as a component of the complex signal transduction chain required to induce the re-programmation of the gene expression pattern, cellular metabolism and totipotency required for the morphogenic competence of somatic cells. In the present investigation optimization of different conditions for *in vitro* morphogenesis from groundnut cultivar JL-24 de-embryonated cotyledon (DEC) explants has been standardized and the different ontogenic stages have been characterized using biochemical determination of some of the antioxidative enzymes and histological studies. Effect of different growth regulators, orientation and size of explants, different nutrient media, organic formulations, carbon source and gelling agents were studied on *in vitro* regeneration. From the studies it was concluded that MS medium supplemented with 5.0 mg l^{-1} BAP and 2.0 mg l^{-1} 2, 4-D with 3.0% sucrose and 0.8% agar proved best as standard regeneration (SR) medium for DEC explants. For biochemical and histological analyses in DEC explants, four ontogenic stages (I-IV) were selected. Antioxidative enzymes like peroxidase (POD) and superoxide dismutase (SOD) were assayed. Polyphenoloxidase (PPO) activity was also assayed as they function in oxygen scavenging by oxidation of phenols. The activities of POD and PPO increased during early stages of morphogenesis and maximum activity was recorded during stage II corresponding to meristemoid formation. A gradual decrease in the activity of both the enzymes were observed during later stages. The activity of SOD showed an inverse trend with low activity during early stages of morphogenesis which peaked during stage III corresponding to formation of organized shoot buds. It is proposed that *in vitro* somatic embryogenesis is favoured by a certain level of oxidative stress characterized by increased activity of SOD and decreased activity of POD resulting in accumulation of H_2O_2. Whereas shoot organogenesis require lower level of oxidative stress which is achieved by scavenging H_2O_2 by increased activity of POD and decreased production of H_2O_2 by low activity of SOD. The oxygen in turn is scavenged by PPO rather than SOD. The activity of the antioxidative enzymes in the study indicated that the mode of morphogenesis was *via* shoot organogenesis. Histological studies of the various stages further supported the correlation between activity of antioxidative enzymes and mode of regeneration.

PP-280
Earthworm assisted bioremediation of some organic waste

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ABSTRACT

The present work evaluates the potential of an epigeic earthworm *Eisenia foetida* to compact the different wastes such as flower waste (Rose, Marigold from local temples) and fruit peel waste (Pineapple, sweet lemon from Local Market shop). These wastes were mixed with cow dung in a ratio of 1:2 (One part organic waste + 2 part cow dung). Two different treatment groups were prepared for vermicomposting and composting: (i) Cow Dung + Rose (CR) (2:1) and (ii) Cow dung + Marigold (CM) (2:1). The end product in vermicomposting shows better stabilization of organic waste compare to conventional composting. Vermicomposting trials resulted an increase in total kjeldahl nitrogen (76.62% - 176.44%); available phosphorus (46.23% - 78.12%); exchangeable potassium (10.65% - 25.67%); exchangeable potassium (10.65% - 25.67%); exchangeable calcium (55.91% - 83.54%) and a decline in pH (15.69% - 21.34%); organic carbon (24.44% - 36.07%) of different treatments group.
Thus study shows one of the safest mode of bioconversion of flower wastes in a value added product namely vermicompost through vermicomposting technique.

PP-281

SYNTHESIS AND CHARACTERIZATION OF POLYMALEIMIDE CONTAINING THIAZOLE AND SULFONAMIDE GROUP

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ABSTRACT

Thiazole and sulfonamide group containing polymaleimide was synthesized using N-[4-(Phenyl) thiazole] maleimide and N-[4-(Sulfonamide) phenyl] maleimide monomer. Thermal, solubility and copolymer composition characterization were done. Gradual single step decomposition was observed with high initial decomposition temperature 233°C and 50% weight loss of PTHSPMI sample was observed at 485°C and 49.31% residue was left at temperature of 500°C. The value of activation energy 18.78 KJ/Mol was calculated using Freeman Caroll method by mathematical analysis of thermogram. Both monomer and copolymer were water insoluble. No azeotropic copolymer formation was seen in any one among the nine copolymer samples. Reactivity ratios r_1 and r_2 values were found 0.125 and 2.422 for monomer units. The maximum value of run number (monomer alternations) was found 65.0 for copolymer sample PTHSPMI8.

PP-282

Quinonoid Constituents from *Heterophragma adenophyllum*

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ABSTRACT

The plants of Bignoniaceous family are widely used in various medicinal purposes as anti-diabetic, trypanocidal, molluscicidal, mosquito larvicidal, anti-oxidant, anti-plasmodial, anti-inflammatory, immunostimulant, anti-microbial, anti-depressant, anti-snake venom, anti-cancer, antinociceptive. *Heterophragma adenophyllum* (Bignoniaceae) syn *Haplophragma adenophyllum*, is a tall evergreen ornamental tree grown in tropical and subtropical climates. Its root is prescribed as drink in viper bite and its wood tar used in various skin diseases. Previous work on this plant led to the isolation of a number of naphthoquinone and anthraquinone derivatives from its heartwood.The heartwood of *Heterophragma adenophyllum* has been reinvestigated for further quinonoid constituents. Five rare naphthoquinones namely 3-hydroxydehydroiso-a-lapachone, 5-hydroxydehydroiso-a-lapachone, 3,8-dihydroxydehydroiso-a-lapachone, 5-methoxydehydroiso-a-lapachone and 8-methoxy-dehydroiso-a-lapachone along with lapachol, tecomaquinone-I, adenophyllone, dehydro-a-lapachone, a-lapachone, haploquinone, veratric acid, ß-lapachone, dehydro-iso-ß-lapachone, ß-sitosterol and stigmasterol have been isolated from its chloroform extract. Their structures were established by spectroscopic methods (UV, Mass, IR, ^{1}H NMR, ^{13}C NMR, DEPT, HMBC and HMQC techniques etc.). Mosher's ester method was applied to examine optical purity and absolute stereochemistry of various dehydroiso-a-lapachones.

PP-283

Photoelectrochemical studies of surfactant in photogalvanic cell for solar energy conversion and storage: Rhodamine 6G-EDTA-NaLS system

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ABSTRACT

Photogalvanic cells as a photoelectrochemical device in which solar energy convert into electrical energy via formation of energy rich species that exhibit the photogalvanic effect. They may be energy source for the future, if their electrical performance is increased. Photogalvanic effect was studies in a photogalvanic cell containing Rhodamine 6G-EDTA-NaLS system. The observed cell performance in terms of maximum potential, maximum photocurrent, short-circuit current, power at power point, conversion efficiency and storage capacity in terms of half change time are -1162 mV, 510 µA, 450 µA, 131.60 µW, 1.26 % and 2.8 h, respectively . The mechanism was proposed for the generation of photocurrent in photogalvanic cell. It is also viewed that the Rhodamine 6G-EDTA-NaLS based photogalvanic cell, with additional advantage of low cost and storage capacity, can give electrical output comparable to that for commercially used power property lacking photogalvanic cells.

PP-284

Oxidation of substituted benzaldehyde by 4-methyl pyridinium di chromate: A Kinetic and mechanistic study

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ABSTRACT

Kinetics and mechanism of oxidation of 4-chloro and 4-methyl benzaldehyde by 4-methyl pyridinium di chromate [4-MePDC] has been studied in acetic acid water medium. 4-MePDC is a mild and selective oxidizing agent and soluble in water and many organic solvent [1]. Aromatic aldehyde is an intermediate species for the production of variety of chemicals [2-4].The reaction was carried out in diffused sunlight. The rate of the reaction is first order in [4-MPDC], [Substrate] and [H^+].The effect of the dielectric constant of the medium and the the ionic strength of the medium indicate the reaction to be ion-dipole type. Activation parameters for the reaction have been evaluated from Arrhenius plot by studying the reaction at different temperature and the mechanism is predicted .The addition of ionic salts Na_2So_4 and $NaClO_4$ do not affect the rate constant. Effect of Mn(II) and Ce(III) also observed and free radical absence was proved. A mechanism involving participation of water molecule in rate determining step.

PP-285

A two stage oxidative tranformation of citric acid by pyridiniumdichromate in aqueous perchloric acid media: Kinetic and Mechanistic study

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ABSTRACT

Studies of oxidation processes have many fold advantages not only in living system but also in analytical, commercial, synthetic and industrial fields. Hydroxy acids are biologically important compounds. They involved and oxidized in metabolism and other biochemical reactions. Oxidation of citric acid by pyridiniumdichromate (PDC) in perchloric acid medium has been studied. The qualitative product study was made under kinetic conditions. The gas produced from reaction mixture turned limewater milky indicat ed CO_2.. Formation of acetone was confirmed by spot test [Feigl.1966]. The apparent reaction order with respect to citric acid was found to be approximately zero.Active oxidizing species involved is protonated PDC. First order plot log (a-x) versus time is broken in two straight lines. Some induction period is also observed. An attempt was made to correlate the rate of oxidation with hydrogen ion concentration. Zucker-Hammett, Bunnett and Bunnett-Oleson plots do not conclusively indicate role of water molecules as proton abstracing agent in the rate-limiting step. Effect of concentration of substrate, PDC, $HClO_4$, Mn (II), Ce (III) and ionic strength has been investigated. In case of citric acid rate increases by addition of Mn(II) and Ce(III) ions(Table-2c). Such observations were also reported by Hiran et al. Thermodynamic parameters have been evaluated. Energy of activation is 52.51 and 51.22 kJ mol^{-1} for two successive stages of oxidation. Entropy of activation is low and negative. Although the activation energy does not correspond to C-C bond breaking, but the reaction products indicate C-C bond breaking. Suitable mechanism has been proposed involving complex formation.

PP-286

Electronic Structure Study of Nd and Gd Sesquioxides: A Compton Scattering Study

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ABSTRACT

In the present work, we have studied the electron momentum densities of Nd_2O_3 and Gd_2O_3 using Compton scattering technique. The experiment has been performed using our 20 Ci ^{137}Cs (661.65 keV) Compton spectrometer [1] at an intermediate resolution of 0.34 a.u. The experimental data have been interpreted in term of theoretical Compton profiles, energy bands and density of states. To compute the theoretical Compton profiles, energy bands and density of states, we have used linear combination of atomic orbitals method as embodied in CRYSTAL09 code [2]. On the basis of experimental Compton profiles and Mulliken's population analysis , relative nature of f electrons in both the sesquioxides is also presented.

PP-287

A Compton profile study of bonding in tin chalcogenides

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ABSTRACT

The IV-VI semiconducting compounds with narrow fundamental gap have extensive applications as thermoelectric materials in solar energy panels, light emitting devices, window coatings, infrared detectors and lasers, etc. [1]. We present the Compton scattering study of tin chalcogenides, namely SnS and SnTe using our 20 Ci ^{137}Cs spectrometer [2] at an intermediate resolution of 0.38 a.u. First principles linear combination of atomic orbitals (LCAO) method [3] is used to compute the respective theoretical Compton profiles, energy bands and density of states. Moreover, covalent nature of these compounds is compared by scaling the Compton profiles on equal-valence-electron-density and it predicts more covalent nature of SnTe than SnS which is in tune to Mulliken's population analysis

PP-288

Synthesis of 3-(4-substitutedphenyl)-6,6-diphenyl-3,3a-dihydro-2*H*-imidazo[2,1-*b*]Pyrazolo[3,4-*d*][1,3]thiazol-7(6*H*)-one and 2-amino-4-(4- substitutedphenyl)-7,7-diphenylimidazo[2',1':2,3][1,3]thiazolo[4,5-d]pyrimidin-8(7H)-one and their ethoxyphthalimide derivatives

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ABSTRACT

Benzil (a -Diketone) when reacted with thiourea in presence of ethanolic alkali, condensation followed by pinacole-pinacoline rearrangement result in the formation of compound 5,5-diphenyl-2-thioxoimidazolidin-4-one. Cyclisation of with chloroacetic acid to gave imidazothiazole-3,5-dione fused bicyclic compound . Condensation of methylene entity in thiazolidinone part with various araldehydes yielded arylidene cyclic chalcones 2-(4-substituted benzylidene)-6,6-diphenylimidazo[2,1-*b*][1,3]thiazole-3,5-dione . These acted as key intermediates for dichotomous reaction sequence, In the first path was refluxed with ethanolic hydrazine hydrate yield. Replacement of imine hydrogen of pyrazole by bromoalkoxyphthalimide group was carried out in ethanolic pyridine afforded 2-N-ethoxyphthalimido 3-(4-substitutedphenyl)-6,6-diphenyl-3,3a-dihydro-2*H*-imidazo[2,1*b*]pyrazolo[3,4-*d*][1,3]thiazol7(6*H*)-one . In another route were refluxed with guanidine nitrate contained ethanolic alkali which gave corresponding 2-aminopyrimidene derivatives. These were further derivatized with our ongoing functionality the bromoalkoxyphthalimide using K_2CO_3 as base in acetone as refluxing media to gave final compound. Structures of synthesized compounds have been assigned on the basis of their analytical and spectral studies. These synthesized compounds were processed for antifungal and antibacterial activity.

PP-289

SYNTHESIS AND BIOLOGICAL ACTIVITY OF IMIDO ESTERS OF 2-ARYL-3-NICOTINAMIDO-4-OXO-1, 3- THIAZOLIDINE-5-YL ETHANOIC ACID

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ABSTRACT

Nicotinic acid hydrazide was prepared by the esterification of nicotinic acid followed by treatment with hydrazine hydrate, which on condensation with various aldehydes (a-e) gave N'-[arylmethylene]nicotinohydrazide (a-e). These on cyclization with mercaptosuccinic acid, yielded 2-{2-aryl-3-(nicotinamido)-4-oxo-1,3-thiazolidin-5-yl}acetic acid (a-e). This Compound (a-e) were further converted into acid chloride derivatives (a-e) by reaction with thionyl chloride. Subsequent treatment of acid chloride derivatives (a-e) with N-hydroxyphthalimide in the presence of TEA furnished the title compounds (a-e). Final compounds have been evaluated for antifungal and antibacterial activity. Some of the compounds have shown significant inhibition towards bacterial and fungal growth.

PP-290

Synthesis and antimicrobial evaluation of some ethoxyphthalimide derivatives of 3-(substituted phenyl)-4-methyl-3a, 6-Di hydropyrazolo[3,4-c] pyrazol-2(3H)-yl (pyridin-3-yl)methanone

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ABSTRACT

5-Methyl-2,4-dihydro-3*H*-pyrazol-3-one reacted with substituted benzaldehyde (a-d) in the presence of anhydrous sodium acetate to gave corresponding 4-arylidene- 5-methyl-2,4-dihyro-3*H*-pyrazol-3-ones (a-d). Further condensation of 4-substituted pyrazolones (a-d) with 2-bromoethoxy-1*H*isoindole- ,3-(2*H*)-dione in the presence of pyridine as a base furnished 2-[2-(4-arylidene-3-methyl-5-oxo-4,5- dihydro-pyrazol-1-yl)ethoxy]-isoindole-1,3-diones (a-d), which on cyclisation with Nicotinohydrazide afforded titled compounds 6-*N*- ethoxyphthalimido-3-(substituted phenyl)-4-methyl-3*a*,6-dihydro pyrazolo[3,4-*c*]pyrazol-2(3*H*)-yl(pyridin-3-yl)methanone (a-d). All the synthesized compounds have been characterized by elemental analysis and spectral data and were screened for various antimicrobial and antiviral activities.
keywords: pyrazolo[3,4-*c*]pyrazoles, Cytotoxicity, Nicotinohydrazide, Antibacterial activities, Antiviral activities.

PP-291

POLAROGRAPHIC STUDY OF COBALT (II) COMPLEX OF 3-HYDROXY-3-M-TOLYL-1-P-SULPHONATO (SODIUM SALT) PHENYL TRIAZENE

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ABSTRACT

Polarographic Study of Cobalt (II) Complex of 3-Hydroxy-3-m-tolyl-1-p-Sulphonato (sodium salt) phenyltriazene has been done in aqueous media at d.m.e in Britton-Robinson Buffer between the pH range 7 – 7.5. The polarographic characteristics diffusion controlled nature, half wave potential ($E_{1/2}$), number of transferred electrons and co-ordination number and stability constant values have been determined. The overall stability constant value found to be log ß11.7.

PP-292

Mechanochemical synthesis and characterization of Cu(II)-hydroxytriazene complex

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ABSTRACT

The studies on metal complexes of hydroxytriazene have been attempted in our laboratory since last many years.[1] In the present paper an attempt has been made to prepare complexes by mechanochemical grinding.To synthesize Cu(II) hydroxytriazene metal complex, Copper Sulphate pentahydrate (.2996gm) and 1,3-diphenyl hydroxytriazene (0.426gm) in stoichiometric amount (1:2 , M:L), the mixture was ground for 2 to 3 hours continuously in mortar & pestle manually .This resulted into formation of dark brown coloured complex .The prepared complex was analysed and characterized by melting point , by TLC , CHN analysis , IR and NMR spectra .The results for synthetic as well as mechanochemical route have been compared and corroborated proving formation of Cu(II)-hydroxytriazene complex through mechanochemical route.

PP-293

"Greener " Mechanochemical Synthesis Of Iron-Hydroxytriazene Complexes

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ABSTRACT

Iron-hydroxy triazene Complexes have been extensively studied during last many years. Review of literature reveals that no attempt has been made to synthesize these complexes through mechanochemical route which has recently attracted much attention.[1] In view of this, present study centres on synthesis of Iron–hydroxytriazene complexes through mechanochemical route. 1,3-diphenyl hydroxytriazene (1.616gm) and iron nitrate nonahydrate(1.278gm) were taken for preparing the complex.The mixture taken in stoichiometric proportion was grinded for 2-3 hours in electric morter pestle .The complex so obtained as detected by change into dark green colour was purified , recrystallized and subjected to physical and chemical characterization. The IR data and C,H,N analysis corroborated with the synthetic sample proving formation of Iron-hydroxytriazene complexes through mechanochemical route.This is first attempt to prepare Iron-hydroxytriazene complexes mechanochemically which is a green synthesis.

PP-294

"BIO-MEDICAL APPLICATION OF NANO-TECHNOLOGY"

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ABSTRACT

21st century's two most promising technologies are biotechnology and nanotechnology.
This science of nanoscale structures deals with the creation, investigation and utilisation of systems that are 1000 times smaller than the components currently used in the field of microelectronics. Biotechnology deals with metabolic process with micro-organisms. Convergence of these two technologies results in growth of nano-biotechnology. This interdisciplinary combination can create many innovative tools. The biomedical applications of nanotechnology are the direct products of such convergences. However, the challenges facing scientists and engineers working in the field of nanotechnology are quite enormous and extraordinarily complex in nature. Utility of nanotechnology to biomedical sciences imply creation of materials and devices designed to interact with the body at sub-cellular scales with a high degree of specificity. This could be potentially translated into targeted cellular and tissue-specific clinical applications aimed at maximal therapeutic effects with very limited adverse-effects. Nanotechnology in biomedical sciences presents many revolutionary opportunities in the fight against all kinds of cancer, cardiac and neurodegenerative disorders, infection and other diseases. This paper presents an overview of some of the applications of nanotechnology in biomedical sciences.

PP-295

KINETIC STUDY OF CO-OXIDATION OF ISOPROPYL ALCOHOL WITH EDTA BY PYRIDINIUMFLUOROCHROMATE

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ABSTRACT

Kinetic study of the co-oxidation of Ethylenediaminetetraaceticacid (EDTA) with Isopropyl alcohol (IPA) by pyridiniumfluorochromate (PFC) has been investigated in the presence of perchloric acid-water medium at 303 K. The reaction is carried out in pseudo first order condition. The rate of co-oxidation of EDTA and IPA is ten times greater than the rate of addition of both compounds separately; EDTA catalyzed the oxidation of IPA. Free radical test proved two electron transfer oxidation and product is Cr (III). Thermodynamic parameter, individual order has been determined. Energy of activation of co-oxidation is 42.52 Kcal. mol^{-1}, while individual is 67.55 Kcal. mol^{1} for IPA & 69.71 Kcal. mol^{1} for EDTA. Probable mechanism has been suggested.

PP-296

SOLVENT FREE SYNTHESIS OF DIFFERENT SUBSTITUTED SULPHUR CONTAINING CHALCONE AND PYRIMIDINE UNDER MICROWAVE IRRADIATION AND THEIR BIOLOGICAL EVALUATION

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ABSTRACT
In the family of of heterocyclic compounds nitrogen and sulphur containing heterocycles are important class of compounds in medicinal chemistry. Pyrimidine, being an integral part of DNA and RNA,imparts to diverse pharmacological properties. As effective bactericide, fungicide, vermicide, anticancer, antiviral agent[1].certain pyrimidine derivatives are also known to display antimalarial, antifilarial and antileshmainal activity[2]. In our present study we have synthesized a new series of sulphur containing chalcone(3a-f) and pyrimidine(4a-e). The advantages of this process is to design and develop new synthetic routes to various bioactive chalcone and pyrimidine which is environmentally desirable and economically viable. The purity was determined using TLC and melting points and structural elucidations were carried out by spectral(IR, 1H-NMR, Mass) studies. The synthesized compounds were also used for various biological screening.

PP-297

Enhanced stilbenes production in cell suspension and root cultures of *Cayratia trifolia* grown in shake flasks and bioreactor

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ABSTRACT
Polyphenols like stilbenes, may provide a protective effect against atherogenesis through the inhibition of the oxidation of low-density lipoprotein and the inhibition of eicosanoid synthesis and platelet aggregation. An efficient system was developed for stilbene production using *Cayratia trifolia* cell cultures. Use of an elicitor of higher plant origin (*Cuscuta*) was demonstrated for the first time in the present work. Among different concentrations tried maximum yield of stilbenes was recorded from cells grown in medium supplemented with 200 mg l^{1} *Cuscuta* elicitor, which was ~8 fold higher than the control yield. This yield was further increased to ~50 mg l^{1} (~14 fold in comparison to control cultures) when cell cultures were treated with a combination of *Cuscuta* elicitor at 200 mg l^{-1}, SA at 500 µM and 3% sucrose. In this case piceid increased to ~ 200 fold and resulted in a productivity of 3.3 mg $l^{-1}d^{-1}$ total stilbenes. This optimized medium was used for further work to develop scale-up technology using a lab made bioreactor. Another higher plant originated elicitor used was gum ghatti (*Anogeissus latifolia,* gum Dhawra). Enhanced accumulation of 8.0-9.0 folds was recorded in stilbenes accumulation and yield over the control by addition of 50 mg l^{1} Gum ghatti. Further extending the effect of biotic elicitors, two fungal elicitors *Fusarium* extract (FE) and *Helminthosporium* extract (HE) were also tried. Increasing concentration of FE in the medium resulted in increased stilbenes accumulation, the optimal concentration being 1000 mg l^{1}. This increase in yield of stilbenes was ~5 times (9.30 mg l^{1}) higher than control value. The higher content and yield of stilbenes have been achieved in root cultures (12 fold) of *C. trifolia* by the combined treatment of elicitor and precursor or alar over control cultures as well as ~8 fold increase over natural roots. This was possible by use of 6% sucrose along with these effectors.India being major producer of medicinal plants, their extracts and to certain extent pure active principles, several plant species has become endangered or is vulnerable to complete eradication. Biotechnological methods are helpful in establishing plant propagation protocols, and production of bioactive molecules through cell cultures. We have achieved enhanced stilbenes accumulation through diverse elicitors' treatment and reported for the first time a preparation from a higher plant parasite *Cuscuta* which can elicit accumulation of stilbenes.

PP-298

FORMULATION AND CHARACTERIZATION OF RAMIPRIL LOADED NANOPARTICLES

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ABSTRACT

Nanoparticles represent a promising drug delivery system of controlled and targeted drug release. They are specially designed to release the drug in the vicinity of target tissue. The nanoparticles have a higher surface-to-volume ratio as compared with bulk material, and therefore the dose and frequency of administration would be reduced hence increasing patient compliance. The aim of this study was to prepare PLGA nanoparticles containing Ramipril by using Nanoprecipitation method. Ramipril is an antihypertensive drug. The size and shape of Nanoparticles prepared characterized by Photon-correlation spectroscopy (PCS), Zetapotential, Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). Nanoparticles have become an important area of research in the field of drug delivery, because they have the ability to deliver a wide range of drugs to varying areas of the body for sustained periods of time.

PP-299

Natural Products in Drug Discovery Research

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ABSTRACT

Osteoporosis, a silent epidemic, is characterized by decreased bone mineral density (BMD), increased risk of fractures and is associated with micro architectural deterioration[1] of bone tissue that results in low bone mass. Natural products for the management of osteoporosis are largely phytoestrogens which include isoflavones, lignins, flavonoids, and coumestans that share structural and functional similarities with naturally occurring or synthetic estrogens. Phytoestrogens exhibit estrogen-like effects at various reproductive and non-reproductive tissues. Traditional medicines have been re-evaluated by clinicians because these medicines have fewer side effects and because they are more suitable for long-term use as compared to chemically synthesized medicines. Most of plant-derived medicines have been developed on the basis of traditional knowledge in health care and in many cases; there is a correlation between the indications of pure substances and those of respective crude extracts used in traditional medicine.

The objective of this study was to determine the in vitro osteogenic activities of selected medicinal plant used traditionally in India. The compounds isolated from three plants viz. Allophylus serratus, Cissus quadrangularis and Vitex negundo were evaluated for their in vitro osteogenic activities. Primary cultures of osteoblasts were used to determine the effects of these components on osteoblast functions. Five (**4**, **6**, **9**, **12** and **14**) of the fourteen compounds isolated led to increase in osteoblast differentiation and mineralization. These findings lend support to the use of Allophylus serratus, Cissus quadrangularis and Vitex negundo in traditional medicine.

PP-300

Interdisciplinary Approach to Rational Computer Aided Drug Design

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ABSTRACT

The development of computational techniques has given the medicinal chemist a powerful tool to use in the development of drugs. A wide variety of computer programs and methods have been developed to visualize the three dimensional shapes of both the ligands and their target sites. In addition, sophisticated graphics packages also allow the medicinal chemist to evaluate the interactions between a compound and its target site before synthesizing that compound. This means that the medicinal chemist need only synthesize and test the most promising of the compounds, which considerably increases the chances of discovering a potent drug as well as reduces the cost of development. An ideal computational method for lead

discovery should be able to generate structurally diverse leads rapidly and should give the estimates of binding affinities that would correlate with experimental values. The first requirement, that is, generation of chemical diversity in structures, is easily achieved using existing computational resources and algorithms: putative ligands can be either extracted from large databases of compounds, or they can be grown computationally by joining molecular fragments (or atoms) stored in the computer's memory. The second prerequisite, accurate prediction of binding affinities (or, equivalently, binding free energies), has proven to be a much more difficult task. Computational methods that attempt to design leads vary in the nature and in the degrees of the simplifying assumptions they use.[7] Successful application of Computer Aided Drug Design (CADD) has been achieved in the discovery of few potent compounds like, Indinavir (Merck). Ritonavir (Abbott), Saquinavir (Roche) etc.

PP-301

Arsenic bioremediation by indigenous bacteria from arsenic contaminated soil

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ABSTRACT

Arsenic contamination of soil and water is a globally growing environmental problem, thus for human welfare removal of arsenic is of great importance. The objective of this study is to get some insight on how microbes could be exploited in developing bioremediation methods for arsenic contaminated soils used for sustainable agriculture. From different arsenic contaminated soil samples four arsenic resistant strains designated as KUAs1, KUAs2, KUAs3 and KUAs4 were isolated having higher tolerance level of Arsenate (V) ranging from 250 mM to 480 mM and of Arsenite (III) ranging from 15 mM to 20 mM respectively. All have shown varied degree of resistance to some other metals and antibiotics. Quantitative estimation of bioremediation indicates towards the reducing capability of these isolates. Among the four isolates, KUAs1 and KUAs4 are most efficient. KUAs4 showed presence of two plasmids of size 4.5Kb and 1.5 Kb respectively. Molecular biological cause of Arsenic resistance of these isolates is under investigation. By 16S rDNA sequence analysis both KUAs1 and KUAs4 were found to be under Genera *Brevibacillus*, species identification is being carried out as the strains showed some distinguishing features. KUAs1 can produce IAA *i.e* it has plant growth promoting features. Other plant growth promoting features are also being tested. Apart from As(V) reduction all the four isolates showed varied degree of As adsorption. So the isolates may provide high hope for harmless and cost effective measures for bioremediation or rhizoremediation of arsenic.

PP-302

KINETICS AND MECHANISM OF OXIDATION OF AMINO ACID (VALINE) BY PBC

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ABSTRACT

Pyridinium bromochromate (PBC) oxidation of amino acid (Valine) yields corresponding aldehydes in the presence of perchloric acid and acetic acid. The reaction is first-order in [PBC] and inverse order in [H]+ ion. Rate increase with increase in amino acid concentration and follows Michaelis-Mentene kinetics i.e. oxidation proceeds via complex formation. While the rate decreases with increase in [H]+ suggest protonated amino acid is non reactive. A study on
the primary kinetic hydrogen isotope effect and solvent isotope effect suggest that C-H and O-H stretching frequencies are affected in the transition state. Activation parameter for the rate determining step has been evaluated. Linear relation between enthalpy change and entropy change suggest all the amino acids taken for study follow similar mechanism. Rate behavior in different solvent composition suggests ion dipolar interaction.

PP-303

CHEMOPROFILING OF *FICUS RELIGIOSA* LINN. (STEM BARK)

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ABSTRACT

Chemo-profiling of herbal drugs represent a comprehensive qualitative approach for the purpose of species authentification, evaluation of quality and ensuring the consistency and stability of drugs and their related products. *Ficus religiosa* Linn. has been used in Ayurvedic medicine for the treatment of ulcers, various skin diseases and scabies and in treatment of diabetes. All plant parts are useful in diseases of blood vagina, uterus, given in leucorrhoea, burning sensation and biliousness. It contains many phytochemical such as phenols, tannins, steroids, alkaloids and flavonoids, ß-sitosteryl-d-glucoside, vitamin K, n-octacosanol, methyl oleanolate, lanosterol, stigmasterol, lupen-3-one. TLC were performed for preliminary identification of constituent in solvent system Toluene:Chloroform:Acetone (40:25:35 v/v/v), gallic acid was used as standard for phenolic compound. Phenolic compound was estimated in alcoholic extract of *Ficus religiosa* Linn. (stem bark) by high performance thin layer chromatography (HPTLC). Precoated silica gel 60 F 254 (E. Merk) TLC plates were used as stationary phase and Toluene: Chloroform: Acetone (40:25:35 v/v/v) was used as mobile phase. Detection and quantification were performed by densitometry at ? 254 nm. The linear range was 200 ng to 600 ng. This HPTLC method was found to reproducible, accurate and precise.

PP-304

Comparative study of hypolipidemic profile of resinoids of *Commiphora wightii* / *Commiphora mukul* from different agro-climatic zones

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ABSTRACT

The anti-hyperlipidemic activity of resinoids of guggul (*Commiphora wightii* / *Commiphora mukul*), belonging to family Burseraceae (Genus: *Commiphora*), collected from different parts of India, was studied on cholesterol-rich high fat diet (HFD) induced model of hyperlipidemia in rats. The exudates of guggul were collected from Gujarat, Madhya Pradesh and Rajasthan (India), falling in three different agro-climatic zones i.e. 'Gujarat plains and hills region', 'Eastern plateau and hills region' and 'Western dry region' respectively. The resinoids of these exudates were prepared in ethyl acetate (moderately non-polar) and ethyl alcohol (highly polar) using solvent extraction methods. The physico-chemical characterization of these resinoids was carried out to determine their appearance, yield %, moisture %, ash %, acid value (mg/KOH/g), saponification value (mg/KOH/g), ester value and iodine value (g/g). Anti-hyperlipidemic study was carried out on all resinoids in HFD induced model of hyperlipidemia in Wistar Albino rats. The comparative study of anti-hyperlipidemic activity of guggul collected from different agro-climatic zones demonstrated that the resinoids of exudates of *Commiphora wightii* and *Commiphora mukul* collected from Gujarat and extracted in ethyl acetate and the resinoids of exudates of *Commiphora mukul* collected from Madhya Pradesh and extracted in ethyl acetate possessed significantly higher anti-hyperlipidemic activity compared to other resinoids. It appears that the bioactive metabolites present in plant extracts are more soluble in ethyl acetate, indicating superior activity than alcohol. However, subsequent studies on fraction level and isolation of active ingredients from these exudates are required to be undertaken for determining the reasons for variation in their activity.

PP-305

DEGRADATION OF CRYSTAL VIOLET USING COPPER MODIFIED IRON OXIDE AS HETEROGENEOUS PHOTO - FENTON REAGENT

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ABSTRACT

The heterogeneous photo-Fenton degradation of crystal violet under visible light has been investigated using copper modified iron oxide. The photocatalyst has been prepared by coprecipitation method. The rate of photocatalyic degradation of dye was monitored spectrophotometrically. It has been observed that photocatalytic degradation follows pseudo first order kinetics. The effect of various parameters like pH, concentration of dye, amount of photocatalyst, amount of H_2O_2 and light intensity on the rate of photo- Fenton degradation has also been observed. Photocatalyst has been characterized by IR spectroscopy, scanning electron microscopy and X-ray diffraction. Chemical Oxygen Demand (COD) of the reaction mixture before and after exposure was determined. A tentative mechanism for the photocatalytic degradation of crystal violet has also been proposed. Involvement of $^{\bullet}OH$ radicals has been confirmed by using isopropanol and butylated hydroxy toluene (BHT) as $^{\bullet}OH$ radical scavengers. It has been observed that rate of reaction is drastically reduced in the presence of these scavangers. Under similar conditions Fe_2O_3 has also been prepared. The efficiency of Fe_2O_3 and copper modified Fe_2O_3 has been compared for the photocatalytic degradation of crystal violet. Heterogeneous photo-Fenton degradation of crystal violet has been carried out with modified iron oxide under visible light. Under optimal conditions in the presence of Cu-modified Fe_2O_3, rate of degradation of the dye is found to be 2.87×10^{-4} s^{-1}, while in presence of pure Fe_2O_3, the rate of photo-Fenton degradation is found to be 2.16×10^{-4} s^{-1}.

PP-306

Transportation of Nickel and its intracellular compartmentalization in a Ni resistant bacterial isolate *Bacillus thuringiensis* KUNi1

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ABSTRACT

Microbial interaction with metallic elements is a frequent event that often leads to intracellular accumulation of these cations from their environment. Although very low levels of several metals are essential, microorganisms show cation uptake, utilizing various mechanisms often at concentrations high enough to be detrimental to them, in selected cell sectors and/or convert them to a more innocuous form such as insoluble phosfide, sulphide, carbide or hydroxide deposits. This localized metal sequestration through binding with various detoxifying ligands has been evolved as an effective microbial strategy to counteract toxic cations. A isolate of *Bacillus thuringiensis*, named as KUNi1 from industrial waste was characterized in terms of Ni^{+2} sensitivity and the mode/ extent of its accumulation as regulated by selected factors. This study explored the intracellular compartmentalization of Ni^{+2} in KUNi1, using transmission electron microscopy and energy dispersive X-ray analysis (EDXA). Simultaneously, X-ray powder diffraction (XRD) analysis was also used to ascertain the chemical nature of sequestered metal in this bacterium. Nickel is a component of hydrogenase enzyme and activity of this enzyme was found to be increased in presence of Ni (II) in the growth medium up to an optimal level. Mg^{+2} was found to be significantly inhibiting Nickel transport in this isolate. This inhibition can be relieved by increasing the level of Ni^{+2} in the assay buffer. Ni^{+2} transport is significantly inhibited by respiratory inhibitor like azide, showing that Ni^{+2} transport in *Bacillus thuringiensis* KUNi1 is probably energy dependent.

PP-307

Synthesis of ?–Butyrolactone Derivatives as Possible Spermicide

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ABSTRACT

?–Butyrolactone ring constitute a very important structural component of organic compounds as it is present in about 10% of all natural products. These lactones have an impressive biological profile including strong antibiotic (e.g. Xanthatin), antifungal (e. g. Encelin), antihelmitic, antitumor, antiviral, antiinflammatory and cytostatic properties[1]. Several a,ß-unsaturated ketones have been proved to possess a wide spectrum of biological activity, including anti-tumour activity that has been attributed to reactivity towards cellular thiols[2]. 17 novel water soluble butyrolactone derivatives were synthesised and screened for spermicidal activity. 2-Acetybutyrolactone (3-acetyldihydrofuran-2(3H)-one) is an active methylene compound, which was C-alkylated by refluxing it with potassium carbonate and aminoalkyl chlorides hydrochlorides in acetone. The resulting compounds **(II-V)** were then converted to water soluble tartarate salts **(1-4)**.Compounds **I-V** were further condensed with aldehydes namely vanillin (4-hydroxy-3-methoxybenzaldehyde), 4-(dimethylamino)benzaldehyde and 4-hydroxybenzaldehyde to yield compounds VI-X (tartarate salt **9-13**) , XI-XV (tartarate salt **9-13**) and XVI-XX (**14-17**) respectively. Tartarate salts of **1-17** were tested for spermicidal activity along with other microbicidal activities.

PP-308

Photoinduced Electron Transfer from Eu(II)-Complexes to Organic Molecules: An Approach to Control the Rate of Back Electron Transfer

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ABSTRACT

Controlling the rate of back electron transfer has achieved significant importance in basic as well as applied science. Present investigation describes a detail analysis of photoinduced electron transfer from Eu(II)-complexes to variety of organic electron acceptors. Rate of the forward electron transfer was monitored with steady state and time resolved luminescence spectroscopy. Rate constants of forward electron transfer are in the range of 10^8~10^9 $M^{-1}s^{-1}$, indicating the high feasibility of the corresponding process. Estimation of electron transfer rate constant using Marcus equation suggests that reorganization energy is comparable with free energy change associated for electron transfer, which results fast forward electron transfer from Eu(II)-complexes. Radical cation and anion were characterized from nano-second laser flash photolysis study. Excited state decay from radical cation and/or anion suggests that back electron transfer rate constants are several order of magnitude less (10^4~10^5 s^{-1}) compared to that of forward electron transfer. Experimentally obtained back electron transfer rate constants are in agreement with theoretically estimated value where reorganization energy largely deviates from free energy of back electron transfer, indicating that activation energy associated with back electron transfer is relatively high, which is evident from the slow back electron transfer process.

PP-309

Preparation and characterization of Polymeric Nanoparticles of Alprazolam

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ABSTRACT

Controlled drug delivery systems and polymeric nanocarriers have undergone significant development in recent years. Polymers like polylactic acid (PLA), polyglycolic acid (PGA), poly (lactic-*co*-glycolic acid) (PLGA), are approved by the World Health Organization (WHO) and Food and Drug Administration (FDA) as materials that can be used in medicine and pharmacy. Owing to their biodegradable, biocompatible and non toxic nature, polymer materials, such as copolymer poly (lactic-*co*-glycolic acid) (PLGA), are widely used in various medical applications. The purpose of this research was to prepare Alprazolam nanoparticles by emulsion-diffusion-evaporation technique using PLGA biodegradable polymer. PVA-chitosan

blend was used to stabilize the PLGA nanoparticles. The nanoparticles were characterized by photon-correlation spectroscopy (PCS), Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). Fourier transform infrared spectroscopy (FTIR) and Zeta potential studies were also performed. Alprazolam belongs to the class of benzodiazepine with anxiolytic, muscle relaxant, an anticonvulsant properties which is generally used as a hypnotic and as a tranquilizer.

PP-310

Synthesis, Anti-proliferative, and c-Src Kinase Inhibitory Activities of Chromone Derivatives

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ABSTRACT

Chromones are known as animportant class of naturally occurring compounds. Chromone derivatives are considered as privileged structures in therapeutics since they possess a wide spectrum of biological activities such as antiproliferative,Sharma et al.[1]antioxidant, antiviral, anti-inflammatory, kinase inhibitory, antihypertensive, anti-allergic and antifungal properties, Khan et al.[2,3]. Molecular mechanisms of anticancer activity mediated by chromones and their derivatives could be attributed to anti-proliferation, induction of apoptosis, cell cycle arrest, promotion of differentiation, inhibition of angiogenesis and various enzymes involved in the signalling pathway, and modulation of multidrug resistance, Ren et al [4]. Our research group has synthesised a series of differently substituted chromone derivatives, all of which are characterized using ^{1}H NMR, ^{13}C NMR, and mass spectrometry. Their anti-proliferative activities were examined against three human cancer cell lines i.e. breast carcinoma (MDA-MB-468), ovarian adenocarcinoma (SK-OV-3), and colorectal adenocarcinoma (HT-29). A few compoundsexhibited modest Src kinase inhibitory activity (IC_{50} = 52-57 μM). Structure-activity relationship studies with respect to the nature and position of substituents on the lead compounds could be further exploited for the design and development of more potent anticancer agents and/or Src kinase inhibitors.

PP-311

Exploring molecular modeling aspects of substituted thiazole/ alkyl oxadiazole benzenesulfonamide as beta-3 adrenergic receptor agonist ligands for anti-obesity drug development

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ABSTRACT

Obesity is a medical condition in which excess body fat has accumulated to the extent that it may have an adverse effect on health, leading to reduced life expectancy and/or increased health problems. Despite the seeming inexorable progression of this disease, there have been limited advances in the pharmacotherapy of this condition[1]. Doubts have been raised on the long-term sustainability of this weight loss. ß$_3$-adrenoceptors agonistcapable of increasing metabolic rates by selective activation of these receptors is considered as a potentially effective approach for the treatment of obesity and diabetes in recent years. The main problem with ß$_3$-adrenoceptor agonists is their cross-reactivity at the ß$_1$ and ß$_2$-receptors. Since obesity is a chronic condition and drug therapy is likely to occur over a prolonged period of time, there is a need to have very selective ß$_3$-adrenoceptor agonists[2,3]. Comparative molecular field analysis (CoMFA) has been a useful technique in designing important 3-dimensional properties associated with the optimum binding of ligands to a binding site. CoMFA samples the differences in steric and electrostatic field surrounding a set of compounds and maps this biological activity. Successful CoMFA, Adv CoMFA and COMSIA models have been generated for the mentioned compounds. Three alignment strategies was adopted in this methods viz. Common structure based fitting, Rigid body field fit alignment using the steric and electrostatic fields and common feature hypothesis. Two structural series of Human β_3-adrenergic receptor (ARs) agonists were used in the studies. All the molecules were divided into two sets; the training set (thirty) and test set (nine). The calculated fields were scaled and subjected to partial least squares analysis. The cross validated r^2 (q^2) was highly significant for all the three alignments but common structure based alignment was the best among these. The best 3D-QSAR model using this alignment were CoMFA (q^2=0.66), Adv CoMFA (q^2=0.569) and CoMSIA (q^2 =0.667). These models showed good correlation between the observed and predicted activity of the training set and test set (r=0.77) and so the studies may be helpful in designing new chemical entities for ß$_3$-adrenoceptor agonists.

PP-312

Toxicological study of CdO nanoparticle on *Escherichia coli*

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ABSTRACT

Released cadmium from the industries is considered as a major threat to the environment due to its toxicity and long retention-time in higher organisms and biomagnification through food chains.[1] Additional hazards are coming up due to the release of nanosized Cd particles, especially CdO nanoparticles (NPs), from the industries involved in manufacturing quantum dots. This article deals with the toxicological study of synthesized CdO NPs (size ~ 22 nm) on *Escherichia coli*. The NPs showed bactericidal activity against *E. coli*. Bacterial cells changed morphological features at sublethal dose to filamentous form with increasing CdO NPs exposure time, resulting in filamentation associated clumping. Severe damage of the cell surface was found in CdO NPs treated cells in AF micrographs. CdO NPs were found to interfere with the expression level of two conserved cell divis ion components, namely *ftsZ* and *ftsQ* in *E. coli* both at transcriptional and translational level. Interference of CdO NPs in proper septum formation without affecting the nucleoid segregation was also observed in confocal micrographs. The elevated intracellular oxidative stress due to CdO NPs exposure seems to be one of the reasons for the changes in cell morphology and expression of division proteins in *E. coli*.[2] Considering ecotoxicological impact of CdO NPs, attention should be taken before releasing such particles into the environment by developing a scientifically defensible fact profile for the purpose of risk assessment.

PP-313

Green Oils Use in Tyre Tread Cap Compound

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ABSTRACT

The global market place is increasingly demanding safe process oils to reduce the environmental impact of tires. The replacement of classified distillate aromatic extracts by non-carcinogenic MES, TDAE, or naphthenic process oils will reduce the PAH emissions. Tyre manufacturers are currently undergoing a period of change which will see the rubber used for tyres reformulated. In recent years authorities in India have become aware that polyaromatic hydrocarbons released as tyres wear down are a threat to the environment. One of the properties is that the oil should be non-carcinogenic. This is defined as an oil with a polyraromatic content of less than 3%, according to IP 346 (a method that measures the amount of DMSO- extractable compounds) and have an MI-value on the Ames test of less than 1. In addition, the content of certain individual polyaromatic hydrocarbons is regulated. A number of alternatives have been developed and this paper will look at three types of low PCA and one regular high PCA Petroleum oils were chemically analyzed. The oils were characterized for different chemical analysis. The data show that the best results are obtained using LPCA. A comparative study has been carried out on SSBR filled with various oils.

PP-314

Chiral separation of centchroman, a non-steroidal contraceptive agent

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ABSTRACT

Centchroman, (INN: Ormeloxifene hydrochloride, I.P.) is once a week non-steroidal oral contraceptive marketed by HLL Lifecare Ltd. Trivanthpuram, in India. In this paper, we are reporting a validated isocratic HPLC method for chiral separation of d- and l-centchroman. This method is capable of base line separation of its d-and l- isomers. HPLC separation was achieved on a Lux 5µ cellulose-1(250 X 4.60 mm) column [phenomenex], at a flow rate of 1 ml/min with detection wavelength 280 nm & 255 nm, using solvent system comprising of Hexane:2-propanol:TEA:MeOH (90:10:0.5:1). Validation parameters such as limit of detection (LOD), limit of quantitation (LOQ), linearity, precision, accuracy, specificity & preformulation studies were conducted according to new guidelines of International Conference on Harmonization (ICH).

PP-315
Synthesis and potential cns activity of some novel 3-[5-substituted 1,3,4-thiadiazole -2 yl]-2- styryl 4(3h) quinazolineones

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ABSTRACT
One of the most frequently encountered heterocyclic in medicinal chemistry is 4(3H)-quinazolinone. In continuation of our work (*Kashaw et al., Eur. J. Med. Chem., 2007, in press*) we synthesised a series of novel 3-[5-substituted phenyl-1,3,4-thiadiazole -2 yl]-2- styryl quinazoline-4(3H)-ones and evaluated for anticonvulsant and sedative-hypnotic. 2-Amino-5-aryl 1' 3' 4'-thiadiazoles (amine) was prepared from cyclisation of thiosemicarbazones of the corresponding aromatic aldehydes in the presence of ferric ions. 2-Methylbenzoxazin-4(3H)-one was refluxed with amine to get 2-Methyl-3-(substituted 1'3'4'-thiadiazole-2'-yl)-4(3H)-quinazolinone. The title compound 3-(5'-phenyl-[1'3'4']-thiadiazol-2'-yl)-2-styryl-quinazoline-43(H)-one (Fig. 1) was obtained by refluxing 2-Methyl-3-(substituted 1'3'4'-thiadiazole-2'-yl)-4(3H)-quinazolinone and aromatic aldehyde in glacial acetic acid. The physicochemical and spectral data were consistent with the title compounds. After i.p. injection to mice at doses of 30, 100, and 300 mg/kg body weight 2-styrylquinazolin-4(3H)-one derivatives were examined in the maximal electroshock induced seizures (MES) and subcutaneous pentylenetetrazole (scPTZ) induced seizure models in mice. The neurotoxicity was assessed using the rotorod method. Out of eighteen compounds only four compounds showed anticonvulsant activity in one or more test models. All except two exhibited significant sedative-hypnotic activity via actophtometer screen. From the experimental observation it can be concluded that synthesized compounds exhibited relatively better sedative-hypnotic. In conclusion the present results have revealed that synthesised 2-styryl-quinazoline-4 (3H)-one exhibited better antibacterial activity than antifungal activity

PP-316
Polysaccharides based nanoparticles: a novel drug delivery system proposed for the macrophages targeting

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ABSTRACT
The purpose of present study was the development and optimization of Amphotericin B bearing dextran sulphate/fucoidan based nanoparticles. The nanoparticles were efficiently prepared via polyelectrolyte complexation method and characterized for particle size, polydispersity and zeta potential. The developed system was optimized for the different process and formulation variables such as ratio of dextran sulphate and fucoidan, concentration of chitosan and tripolyphosphate, and curing time of the nanoparticles. Aggregation of the Amphotericin B within the nanoparticles was confirmed by UV-visible spectroscopy based aggregation study. Hemolytic effect of the developed formulation was evaluated. Further, cellular uptake and cytotoxicity studies were conducted using J774 macrophage cell line. Fucoidan was found to have more impact on the both size and zeta potential on compare to dextran sulphate. Size of the nanoparticles was found to increase with increase on the concentration of the chitosan and tripolyphosphate but after a certain extent impact of tripolyphosphate was found to be negligible. The effect of nanoparticles curing time did not show any statistical differences on the nanoparticles mean size, which suggests a fast complexation between polyelectrolytes. Developed formulation was found to be having a significant less hemolytic activity in comparison to free drug. The negligible cytotoxicity of the developed formulation showed the safety characteristics of the employed excipients. Moreover, there was a significant higher uptake of the nanoparticles by the macrophages on comparison to free drug which in turns open a new hope for the treatment of the infectious disease like visceral leishmaniasis where amastigotes reside deep inside the macrophages.

PP-317

A green route for synthesis of some new cyanopyridenes *via* common intermediate chalcone & their antimicrobial activity

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ABSTRACT

An efficient facile one-pot synthesis of 2amino-3-cyano-4,6-diarylpyridines from a,ß-unsaturated carbonyl compounds (Chalcones) and malononitrile in presence of ammonium acetate using inorganic solid support and solution phase under microwave activation is described. The reaction time has been brought down from hrs to minutes with improved yield as compared to conventional heating methods. This non-conventional synthetic approach using basic alumina as solid support was found superior in comparison to solution phase and environmental acceptability. All the synthesized compounds have been screened for their antimicrobial activity. Structure elucidations of all the synthesized compounds have been accomplished by elemental analysis, IR, ^{1}H NMR and mass spectral data.

PP-318

Dynamics of larval salivary gland protein secretions in the hybrids of *Drosophila nasuta nasuta* and *Drosophila nasuta albomicans*

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ABSTRACT

The larval salivary gland secretory proteins in *Drosophila* are tissue specific and stage specific proteins that are released to the exterior. These secretions are supposed to attach the pupae to the substratum (Lane *et. al*., 1972; Fraenkel and Brooker, 1953; Korge, 1977). *Drosophila nasuta nasuta* and *Drosophila nasuta albomicans* belonging to the frontal sheen complex of *Drosophila immigrans* species group are allopatric sibling species and are cross fertile (Nirmala and Krishnamurthy, 1972). Studies on larval salivary gland secretory proteins in various members of *D. n. nasuta* subgroup have revealed that these proteins are copiously produced during the third larval instar stage and major protein fractions show X linked pattern of inheritance (Ramesh and Kalisch, 1988; 1989). Present experiments were designed to assess the dynamics of protein secretion in the F1 hybrids. Preliminary studies have shown increase in total protein content between the parents and the hybrids with respect to salivary gland secretory proteins.

PP-319

DESIGNING AND CHARACTERIZATION OF COLON TARGETED DRUG DELIVERY OF ORNIDAZOLE

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ABSTRACT

The aim of the present study was to develop colon targeted drug delivery system for ornidazole using microflora activated (Xanthan gum and Guargum) and pH dependent (Acrycoat coating) approach. Matrix tablet of ornidazole containing various proportions of xanthan gum and guar gum (10 to 50%) were prepared by using wet granulation technique and were subjected to *in vitro* drug release studies in simulated GIT condition and *in vivo* roentgenography.

Drug released studies indicated that, 37.98 to 92.9% of ornidazole were released from xanthan gum and guar gum matrix tablets at physiological environment of stomach and small intestine with minimum release in tablet containing guar gum 50 %. Since, the drug release was quiet high within the first 5 h, a further coating was done on matrix tablets containing 50% of guar gum to get envisage objective.

Acrycoat L-100, Acrycoat S-100 and ratio of Acrycoat L-100, S-100(1:1) were used as enteric coating material and level of coating was 10%. At the end of 5h drug release were found 25.96, 1.87 and 11.87% for Acrycoat L-100, Acrycoat S-100, (1:1) ratio of Acrycoat L-100 and S-100 coated tablets respectively. Further at the end of 24 h drug release was found 60.39 to77.99% for different coated formulations.

When the dissolution study for optimized (Guargum 50 % coated with Acrycoat S-100) tablets was continued in simulated colonic fluids, using 10% w/v human faecal slurry, the drug release was increased from 60.39% to 98.6%, indicating the susceptibility of the Guargum formulations to the anaerobic faecal bacteria.

Furthermore above optimized formulation subjected to *in vivo* roentgenography study in dog which also strongly supported deformation of tablet in colon. The study revealed that Acrycoat S-100 coated Guargum (50%) tablet was most likely to provide targeting of Ornidazole for local action and; can be promising vehicle for targeted drug delivery to colon.

PP-320
A Comparative Study of Binding Ability of Ionic Surfactants with an Antidepressant Phenothiazine Drug

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ABSTRACT

The excess amount of drugs can cause over-stimulations, psychotic illness and other disorders, so the targeted drug-delivery in body organs is necessary and for these purpose surfactants can be used as drug-carriers.[1-3] Also the micelles can solubilise poorly soluble drugs in their hydrophobic core, thus increasing their bioavailability. Further, they can stay in the blood long enough and their sizes allow them to accumulate in areas with leaky vasculature.[4] In addition to all this, drug-surfactant mixed systems have gained economic importance as the micelles are easy to prepare on large scale.[4] The present work deals with the effect of ionic surfactants, sodium dodecylsulphate (SDS), dioctylsulphosuccinate sodium salt (AOT), dodecyltrimethylammonium bromide (DTAB), didodecyldimethylammonium bromide (DDAB) on the physicochemical properties of antidepressant phenothiazine drug, trifluoperazine dihydrochloride (TFP). Surface tension, fluorescence and electronic absorption measurements have been done in order to study the nature of interactions between drug-ionic surfactants mixtures. Various interfacial, micellar, spectroscopic and corresponding thermodynamic parameters have been calculated from these techniques. The values of interaction parameter (ß) suggests that cationic surfactants exhibit less synergistic interactions with TFP as compare to anionic surfactants. To confirm this we further performed the fluorescence quenching and electronic absorption titrations of ionic surfactants with TFP. Anionic surfactants (SDS, AOT) have been observed to bind preferentially with TFP than cationic surfactants (DTAB, DDAB) which supports the presence of cationic charge on the head group of drug and signifies that anionic surfactants can act as better drug-carriers than cationic surfactants even at very low concentrations. The blue shift and decrease in fluorescence intensity observed in fluorescence quenching methods for TFP+ SDS/AOT mixtures confirms the formation of new complex between interacting species. Also the number of binding sites for drug molecule has been estimated which helps to insight the mechanism of the drug-surfactants complexes formed. The results indicate that among electrostatic, hydrophobic and van der Waals forces, former one are the predominant intermolecular forces between TFP and ionic surfactants.

PP-321
Heavy Metal Tolerance and Antibiotic Resistance Patterns of *Pseudomonas aeruginosa* Isolated From Soil of Zawar Mines Udaipur, India

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ABSTRACT

A number of interactions between microbes and metals have important environmental and health implications. Some implications are useful and some are not as beneficial, as the presence of metal tolerance mechanisms may contribute to the increase in antibiotic resistance [1]. The heavy metal tolerance and antibiotic resistance patterns of two strains namely *Pseudomonas aeruginosa* HMR1 and *P. aeruginosa* HMR16 isolated from soil of Zawar Mines, Udaipur were studied. Minimum inhibitory concentration (MIC) of the heavy metals - zinc, chromium and nickel were studied by inoculating the isolates aseptically on nutrient agar plates, supplemented with different concentrations (mM) of the heavy metals: Zn (0.0- 15), Cr (0.0- 0.35) and Ni (0.0-10). The Kirby-Bauer disc diffusion method was used to obtain antibiotic resistance patterns. Both the isolates showed MIC of 10 mM, 0.25 mM and 1 mM for Zn^{+2}, Cr^{+6} and Ni^{+2} respectively and exhibited resistance towards several antibiotics including broad spectrum antibiotics, ß-lactam, glycopeptide and cephalosporin. However both the isolates were susceptible towards some commonly used antibiotics belonging to rifamycin, aminoglycosides and polymyxin. The above studies have shown the dual properties of the bacterial genome in rendering the heavy metal tolerance as well as antibiotic resistance.

PP-322

In vitro propagation of ayurvedic medicinal herb centella asiatica

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ABSTRACT

Centella asiatica is valuable ayurvedic medicinal herb belong to family apiaceae. The present research work was demonstrated *in vitro* propagation of *C. asiatica* using various explants viz, apical shoot proliferation and nodal segment of mother plant. These explants were inoculated on MS (Murashige and Skoog 1962) medium supplemented with different concentration of phyto-hormones like, BAP (Benzyl amino purine); KIN, IBA and IAA (indol -3-acetic acid) produce maximum percentage of multiple shoots. Apical shoot and nodal explants inoculated on MS medium supplemented with various concentrations of KIN 0.2, 0.4, 0.6, 0.8, 1.0 mg/l, BAP 0.4, 0.8, 1.2, 1.6 mg/l with combination of 0.2 mg/l IBA and IAA gives average percentage of shoot multiplication. Highest shoot multiplication was observed 1.6 mg/l BAP in combination of 0.2 mg/l IBA. BAP most affected on shoot multiplication as compare to KIN and any other combination of KIN was also recorded.

PP-323

Enzymatic Biosensors – Characterization and Applications in Biopharmaceuticals

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ABSTRACT

Enzyme immobilizations onto matrices which are economical, environmentally safe and biodegradable, have gained much importance in foods, cosmetics, biomedical and pharmaceuticals applications. Biopolymers, such as alginate, chitin, chitosan and agar, have found to be suitable matrices for enzyme immobilization. The goal is to check the suitability of enzyme-entrapped beads for the preparation of the enzyme biosensor electrode. The work is significant because of its potential use in environmental and biochemical sciences, and pharmaceutical industry. For example, such enzyme biosensors can be utilized to measure levels of trace elements in environment and biological specimens. Urease, which catalyses the hydrolysis of urea to ammonia and carbon dioxide, is used in an immobilized form in kidney machines for the purpose of blood detoxification. Immobilization of urease is also carried out in several matrices for various analytical and clinical applications. Furthermore, several biosensors with immobilized ureases are used to efficiently assay blood urea. These include a recent method of entrapment of urease inside reversed micelles as a method of immobilization and using a glass electrode as a sensor.

In view of the above application, it was aimed at further developing the enzyme biosensor electrodes that are based on immobilized urease-alginate beads. For this purpose, urease was extracted from the seeds of pigeon pea (*Cajanus cajan L.*) and then urease enzyme was tested and entrapped in calcium alginate beads. Notably, Calcium alginate has been used to entrap enzymes (pigeon pea urease) because this method is found to be economical, safe and convenient .The kinetic properties of soluble urease was compared with the immobilized enzyme. The immobilized urease showed a shift in its optimum pH from 7.5 to 7.0 in Tris/acetate buffer. Optimum temperature also shifted from 47^{o}C to 65^{o}C compared with the soluble enzyme. Alginate-immobilized pigeon pea urease was observed to have a higher K_m than that of the soluble enzyme. Moreover, the attempt was made to use immobilized beads for the preparation of a urea biosensor, which has been developed from potentiometric pH glass electrode coupled to a calomel electrode. Then, by using the enzyme biosensor electrode, serum urea has been estimated. Now, ongoing and future work would show that urea biosensor will be able to detect urea with good linearity and reasonable sensitivity. In short, immobilized enzymes have biomedical and industrial applications and for this reason, this area has continued to develop into an ever-expanding and multidisciplinary field.

PP-324

H-Point Standard Addition Method for Simultaneous Determination of Copper (II) and Cobalt (II) Ions

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ABSTRACT

A new, simple, inexpensive and sensitive method for the simultaneous spectrophotometric determination of Cu(II) and Co(II) by H-Point Standard Addition method has been reported . 3-Hydroxy-3-(4-Methyl Phenyl) -1-(3-Chloro, 2- Methyl Phenyl)Triazene(HMCPT) was used as reagent at pH 6.7. This method is based on the difference in the absorbance of yellow complexes of above reagent with Cu(II) and Co(II) at different wavelength pairs. The result showed that Cu(II) and Co(II) can be determined simultaneously with concentration ratio of 3:1 and 1:3. This method was successfully applied to the determination of these metals in synthetic samples.

PP-325

Simultaneous spectrophotometric determination of iron (III) and copper (II) ions by H-point standard addition method

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ABSTRACT

Simultaneous spectrophotometric determination of Fe(III) and Cu(III) has been described using H-point standard addition method (HPSAM).This method is based on the difference in the absorbance of 3-hydroxy-3-phenyl-1-[2,5-dichlorophenyl] triazene(HPDCT) complexes with Fe(III) and Cu(II) at pH 5.2 using different wavelength pairs. The result show that Fe(III) and Cu(II) can be determined simultaneously with concentration ratios of 3:1 and 1:3. The proposed method has successfully been applied for simultaneous determination of iron and copper in synthetic samples.

PP-326

Bile Tolerance Ability of *Lactobacillus plantarum* CM1

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ABSTRACT

Lactobacilli are extensively used in the food and pharmaceutical industries as commercial probiotics. Probiotics refer to viable microorganisms that promote or support a beneficial balance of the microbial population of the gut [3]. According to the guidelines of the of probiotic organisms, reported by a joint FAO/WHO working group, bile tolerance is one of the most widely used in vitro tests [2]. It is focused on the assessment of the potential of one putative probiotic strain to overcome the action of bile salts which is present in the upper part of the intestine [1]. The present study aimed at dectection of bile tolerant ability of *Lactobacillus plantarum* CM1 isolated from cow milk. The strain was examined for resistance to 0.1 to 0.5 % of sodium taurocholate and oxgall upto 6 h of incubation period. *Lactobacillus plantarum* CM1 showed moderate tolerance to sodium taurocholate and fairly high tolerance to oxgall. Almost 80% of growth was observed in MRS broth supplemented with 0.5 % of oxgall after 6 h of incubation period. Only 21.4 % of growth was observed in MRS broth supplemented with 0.5 % of sodium taurocholate after 6 h of incubation period. The tolerance of *Lactobacillus plantarum* CM1 to the bile salts especially against oxgall indicates that it can be a promising probiotic.

PP-327

Synthesis and anti-inflammatory evaluation of 2-(methylsulphonyl amino)-4-(arythio/aryloxy) methyl thiazoles

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ABSTRACT

Search of newer and safer non-steroidal anti-inflammatory agents is everlasting as existing drugs likely to be outdated due to clinical overuse or observed side effects. 2, 4-Disubstituted thiazole derivatives have proved their use as anti-inflammatory compounds. There for new 2-methylsulphonyl amino-4-aryloxy methyl thiazoles and 2-(methylsulphonyl amino)-4- (arythio) methyl thiazoles have been synthesized from 2-(methylsulphonyl amino)-4- chloromethyl thiazoles. The precursor 2-amino-4-chloromethyl thiazole hydrochloride has been prepared using Hantzsch synthesis by cyclocondensing 1, 3-dichloroacetone and thiourea in ethanol. Representative synthesized compounds have shown significant anti-inflammatory activity using carrageenan-induced mice paw edema method compared with indomethacin. The details of the synthetic work and bio-evaluation will be presented.

PP-328

Seasonal Study of Physicochemical and Bacteriological Parameters of Pichhola Lake of Udaipur District (Rajasthan), India.

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ABSTRACT

The deterioration of water quality due to pollution is one of the major concerns to environmentalists and monitoring water quality is of significant value in determining the potability of water. Limnology and Microbiology of Udaipur lakes during the year 2004-05 were studied by [1]. Yadav and kumar [2] had monitored water quality of Kosi river in Rampur district, Uttar Pradesh, India. In the present study an attempt has been made to study the water quality of Pichhola lake of Udaipur (Rajasthan), India. Water samples were collected during different seasons like winter, summer and monsoon in the year 2011 for analysis of 7 physicochemical parameters pH, Temperature, total alkalinity, total hardness, dissolved oxygen, BOD and COD. In addition, the bacteriological analysis like total bacterial count, total coliforms and total faecal coliforms were also detected which are the indicator organisms of pollution studies. The results showed that total bacterial counts were found in the range of 30×10^3 to 52×10^3/ml. The range of MPN was found between 350 to 2400/100 ml for coliforms and 75 to 280/100ml for faecal coliforms. The water quality of lake Pichhola of Udaipur is taken into account to ascertain the drinking water supply in Udaipur and bacteriological analysis reveals that the lake water is polluted.

PP-329

Sugar based Crown Ethers: An inexpensive source of asymmetry

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ABSTRACT

Chiral crown ethers are suitable for selective complexations of guest molecules and for the control of enantioselective reactions[1,2]. Stoddart et al.[3] has prepared chiral 18-crown-6 derivative possessing *trans*-tetrahydrofuran-2,5-diylbis(methylene) unit by using 2,5-anhydro-D-mannitol. Examination of framework molecular models indicates that incorporation of a constrained diethyleneglycol unit in the form of either a *cis*- or *trans*-fused tetrahydrofuranyl-2,5-dimethylyl unit into 18-crown-6 constitution can lead to improved orientations of oxygen atoms with respect to the bound cation-metal or guest molecules compared with those observed for complexes of 18-crown-6. Crown ether molecules with saccharide moieties are interesting as chiral phase transfer catalysts[4]. Kinetics of selective transport of alkali metal cations has been reported[5]. All previous reports[6] published on sugar based crown ethers contains only one sugar moiety. In this paper we report the synthesis of chiral crown ether containing two sugar units. In the best of our knowledge this is the first report containing more than one sugar moiety in sugar crown ether containing constrained diethylene glycol units.

Acknowledgement: We thanks IGSTC,Gurgaon for financial assistance. V.K. and R.K. thanks CSIR and UGC New Delhi for the award of Junior research fellowship.

PP-330

Identification of Lactobacilli Isolated From Camel Milk

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ABSTRACT

Camel is a dominant animal in desert areas. Camel milk is the key food in arid and semi-arid areas [1]. Milk contains different type of lactic acid bacteria (LAB). *Lactobacillus* is one of the most important groups of lactic acid bacteria present in camel's milk which can be used in dairy technology. A total of 3 isolates recovered from camel milk sample collected from nearby village of Udaipur district. Genomic DNA of these 3 isolates were extracted and subjected to PCR. PCR was carried out using primer LBLMA-1/R16-1. These 3 isolates showed expected 250 bp product thereby conforming that they belong to the genus *Lactobacillus.* A study of lactobacilli of camel milk would be of immense importance to explore new strains of microbes with good technological properties that can be used in dairy industry.

PP-331

Interaction of PknJ and MmaA4 controls the physiological and pathological properties of mycobacteria.

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ABSTRACT

The identification of the mmaA4 gene, which encodes a methyl transferase required for introducing the distal oxygen-containing modifications of mycolic acids. MmaA4 is required for the synthesis of keto- and methoxy-mycolic acids. The vaccine strain, *Mycobacterium bovis* BCG strain Pasteur (BCG) has a similar mycolic acid profile, but lacks methoxy mycolates. Synthesis of cell wall lipids, particularly mycolic acids, is essential for survival of mycobacteria *in vivo*. Several of the successful antimycobacterial drugs, including isoniazid (INH) or ethionamide (ETH), inhibit enzymes required for mycolic acid synthesis. The *mmaA4* gene was amplified from gDNA of *Mycobacterium tuberculosis* (MTB) using gene specific primers by PCR and amplified products were cloned into expression vector. In *vitro* kinase assay of MmaA4 with PknJ was performed by ADP-glo kinase assay. The transcript levels of pknJ and mmaA4 were determined by quantitative RT-PCR (qRT-PCR) in different stress conditions. Antisense strain of BCG expressing low levels of PknJ displayed fast growth and reduced level of MmaA4.

PP-332

Synthesis and Characterization of Organic Polymer –Poly Indole

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ABSTRACT

In recent years, there has been a growing interest in the development of Advanced Polymeric Materials and Carbon Based Materials. Advanced polymeric materials like, Nitrogen containing Organic polymers like polyindole, polyaniline, polypyrrole, and polycarbazole, etc have significant flexibility in the available chemical structure which can be modified as required. They have the ability to transfer efficiently the electrical charge produced during the biochemical reaction to the electronic circuit. Unique properties of organic conducting polymers like substitution, accompanied by significant changes in conducting, slow degradation rate, redox and spectroscopic properties permits their application as suitable matrix in different bio-sensor constructions.

PP-333

Phytochemistry and Antimicrobial Screening of *Arvea persica*

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ABSTRACT

Arvea persica is a medicinal plant described as one of the best known remedies for bladder and kidney stones, belongs to the family *Amaranthaceae.* It is well distributed in the north temperate zone especially in the Mediterranean region and Asia. It is used for the treatment of Dysentery, Gonorrhea, Kidney disorders and cutaneous infections.

In the present study the antimicrobial activity of *A.persica* were evaluated by using different solvent extracts and some compounds isolated .The finding provide support for the use of this plants in traditional medicine which fulfills the objective of present study to evaluate the potential of this plant to be used in traditional medicine for antimicrobial activity against important microbial infections.

PP-334

Metal modified fly ash catalyst in cyanoethylation process

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ABSTRACT

Fly ash based solid base catalyst synthesized by loading of Mg/M (M=Ca, Al) mixed oxide on acid activated fly ash, using co-precipitation method, was used in the cyanoethylation of methanol to methyl esters in a heterogeneous manner. Fly ash was chemically activated using sulfuric acid followed by thermal activation at 600°C. Chemically activated fly ash was then treated with metal oxides for loading of metal oxides on fly ash surface. The variation of surface and Physico-chemical properties of the fly ash by activation methods resulted in improved basicity and therefore, catalytic activity for base catalyzed reactions. The physico-chemical properties of synthesized Mg/M/fly ash catalyst were monitored by X-ray diffraction method, FTIR spectroscopy, Scanning electron microscopy and Thermo gravimetric study. The increased concentration of silica surface hydroxyl groups on activated fly ash have a major influence on the loading of Mg/M oxides. The catalytic activity of the catalyst was tested in cyanoethylation of alcohol. Mg/M/fly ash was more active than CaO and MgO in the cyanoethylation of acrylonitrile with methanol at 60°C and atmospheric pressure. The activity data indicate that this heterogeneous catalyst is very active, corresponding to high conversion of acrylonitrile. The highest activity was found at molar ratio of 3.8, with a conversion of 74%, whereas MgO and CaO were inactive. Moreover, lixiviation of the active phase was not observed, thus excluding the contribution of the homogeneous catalysis to the studied cyanoethylation process. The catalyst could be easily recovered and reused giving similar conversion up to three reaction cycles indicating its stability under experimental conditions.

PP-335

Fractionation Technique and the Apparent Solidification Time Test for the Detection of Milk Fat Adulteration with Admixture of Foreign Oils and Fats

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ABSTRACT

A new approach for establishing the purity of milk fat using dry fractionation on the basis of crystallization, which enriches the solid fraction with the body fats and hydrogenated fats, and the liquid fraction with vegetable oils, followed by the application of the apparent solidification time (AST) test was adopted for detecting the admixture of foreign oils and fats in milk fat. The AST values of the solid fraction obtained at 20^0C, and solid and liquid fractions obtained at 18^0C for pure cow milk fat, were 2 min 30 s, and 3 min 21 s and 3 min 31 s, while for buffalo milk fat they were 1 min 58 s, and 2 min 47 s and 3 min 10 s respectively. This new approach can detect some mixtures of foreign oils and fats in cow milk fat but not in buffalo milk fat.

P-336

A convenient one pot synthesis of xanthene derivatives using DBSA as an efficient bronsted acid catalyst under microwave irradiation

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ABSTRACT

Xanthenes are an important class of heterocyclic compounds which occupy a prominent place in the field of medicinal chemistry. Recently, these molecules have received significant attention because of their interesting pharmacological profiles such as antimalarial, anti-inflammatory, anti-depressants and antiviral agents. In addition, they are being used as dyes in laser technologies, pH sensitive fluorescent materials for the visualisation of bio molecular assemblies and photosensitizers in photodynamic therapy applications [1]. Thorough literature search revealed that many synthetic procedures have been developed in the past to obtain xanthenes but the design of a simple, economical and efficient synthetic strategy for the construction of these molecules is highly desired.

In continuation of our on-going work to develop efficient methods [2-5] for the synthesis of biologically important molecules, we wish to present a microwave accelerated one-pot methodology for the synthesis of a variety of xanthene analogues using *p*-dodecylbenzenesulfonic acid as an efficient bronsted acid catalyst.

PP-337

Regenerated Cellulose-Poly (acrylamide) Hydrogel Films for Potential Wound Healing Applications: An In-Vitro Study

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ABSRACT

In the present work, regenerated cellulose/poly (acrylamide) films have been synthesized for wound dressing applications. The water absorbency of these films was a function of amount of crosslinker N, N'- methylene bisacrylamide, and cellulose in the feed mixture. The samples, having different compositions, showed Tensile Strength in the range of $9.98x10^5$ to $13.40x10^5$ N/m^2.The percent elongation of the films was abnormally high in the range of 110 to 265. The water vapor transmission rate (WVTR) for various films was found to be in the range of 2.03 to 7.18 $mg/cm^2/h$. These films were loaded with antibacterial drug Miconazole Nitrate and their release was studied in the physiological pH at 37^0C. The release data was found to fit well the diffusion controlled Higuchi model. Finally the films demonstrated fair antibacterial action thus establishing their strong candidature as wound dressing materials. These hydrogels were characterized by FTIR, analysis. Finally hydrogels shows antibacterial and antifungal activity.

PP-338

Protective Effects of Curcumin Against Cadmium Induced Reproductive Toxicity In Male Reproductive System of Swiss Albino Mice

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ABSTRACT

Curcumin a polyphenilic compound obtained from rhizome of *Curcuma longa* has long been attributed with numerous healing properties where as cadmium has been known to cause multifaceted damage to living organisms. In the present study mice previously exposed to cur cumin were administered cadmium and cadmium induced toxicity in terms of histopathological damage and the potency of curcumin to check the damage was assessed and compared with the results of control group.

PP-339

Hepcidin levels in aqueous humor of patients with primary open angle glaucoma

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Purpose: Glaucoma is a multifactorial, progressive optic neuropathy with a characteristic loss of retinal ganglion cells beyond typical age-related baseline loss. Reactive oxygen species play a fundamental role in the pathophysiology of many diseases including glaucoma. The iron-catalyzed formation of reactive oxygen species is a major player in these processes. Hepcidin prohormone (Hep) is an important peptide hormone that plays a critical role in the regulation of iron efflux from numerous cell types. Hep binds to and induces the degradation of ferroportin, a protein for iron efflux. Hep is expressed in Muller cells, photoreceptor cells, and retinal pigmented epithelium in an expression pattern similar to that of ferroportin. The increase in Hep expression correlates with a decrease in ferroportin expression, as well as an increase in oxidative stress and apoptosis, as would be expected from an increase in intracellular iron resulting from decreased iron export. Interleukin-6 (IL-6) is a multi-functional cytokine that regulates immune responses, acute phase reactions, and hematopoiesis, and may play a central role in host defense mechanisms. Studies have identified IL-6 as a possible inducer of Hep synthesis. This study was designed to evaluate the Hep and IL-6 levels in the aqueous humor and serum of patients with primary open angle glaucoma (POAG) as compared to age-related cataract patients.

Methods: Fifteen POAG patients and fifteen age-related cataract patients (controls) were included. Aqueous humor samples were collected from the patients undergoing trabeculectomy and cataract surgery. Aqueous humor samples were immediately stored at -80°C until analysis. Blood samples were also collected before surgery. The Hep and IL-6 levels in both aqueous humor and serum samples were measured by enzyme-linked immunosorbent assay.

Results: The mean aqueous humor Hep concentration in eyes with POAG was significantly higher than controls ($p<0.05$) while there was no significant difference between serum Hep concentration of POAG and the control group. No significant difference was found in aqueous and serum IL-6 concentrations in patients with POAG compared with controls. There were no significant correlations between Hep and IL-6 levels among patients with POAG and the control group.

Conclusion: Our results indicate that aqueous humor Hep concentration is higher in POAG patients and independent from the IL-6 concentration in patients with POAG, suggesting that Hep might represent a bridge protein between local inflammation and the consequent loss of retinal ganglion cells.

PP-340

Title: Nanotechnology Advancements in Medicine and Dentistry

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ABSTRACT

Objective: To review Advancements of Nanotechnology in Medicine and Dentistry.

Contents: Nanotechnology is a multidisciplinary field that covers diverse array of devises derived from engineering, physics, chemistry and biology. The burgeoning new field of nanotechnology, opened up by rapid advances in science and technology creates myriad new opportunities for advancing medicine and dentistry and diseases treatment in human health care. Application of nanotechnology to medicine, physiology, dentistry imply material and devices designed to interact with the body at subcellular (molecular) scales with a high degree of specificity. This can be potentially translated into targeted cellular and tissue specific clinical application designed to achieve maximal therapeutic efficacy with minimal side effects.

Nanodentistry: is the future of dentistry in which every procedures will be performed using equipments and devices based on nanotechnology. All diagnosis and treatment will be given using nano particles which are less than 100nm in size and nano robots using a combination of nano medicine in biotechnology, it will become possible to revolutionise various applications examples: restoration, dentin hypersensitivity and agents of drug delivery etc. Nano particles are known to have properties like enhance resistance to heat, solvents and abrasions. Prospects are bright for aesthetic dentistry due to their small size and light absorption and transparency. Dental nano robots will be used for analgesia, plaque control agent delivery and play a major role in orthodontic therapy. This poster discuss the future of medicine and dentistry with the applied aspects of nanotechnology.

PP-341

Synthesis, cytotoxicity, and structure-activity realationship (SAR) studies of andrographolide derivatives

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ABSTRACT

Cancer remains a major cause of lethality because of high incidence and recurrence. Notably, roughly around 50% of the currently used anticancer drugs were discovered from studies on either natural products or natural products based molecules.[1] In recent past, the potent anti-cancer activities of andrographolide, a major constituent of *Andrographis paniculata* Nees (Acanthaceae) have indeed been established. However, despite its impressive biological activities, the major draw-back of andrographolide is poor water solubility making it difficult to prepare formulations of clinical use. Therefore, various semi-synthetic analogues are being developed and evaluated in order to find out better lead(s). It was shown that C14-ester analogs of andrographolide are more potent (*in vitro*) against leukemia compared to native compound andrographolide.[2] In continuation of our work in this area, we have now designed and synthesized several 14-*o*-halo(I/Br/Cl)acetate derivative of andrographolide and their epoxy (? $^{8(17)}$) analogs as well. Cytotoxicities of all synthesized analogues were measured by using MTT assay in human embryonic kidney cancer cells (HEK 293) and normal monkey kidney cells (Vero) as well. Besides, our compounds were also tested against human breast cancer cell lines (MCF 7) and normal breast epithelian cells (MCF 10A). Among the tested compounds, 14-*o*-iodoacetate and 14-*o*-bromoacetate derivatives of andrographolide showed a significant decrease of cell viability of HEK-293 and MCF 7 cells in dose dependent manner; while these compounds did not show any considerable cytotoxicities against normal cell lines (Vero, MCF 10A). Besides, evaluation of the induction of apoptosis was carried out by DAPI nuclear staining method using fluorescence microscope, and by the expression of the proteins level (PARP, BAX, BCL-XL and P53) using western blot analysis.

PP-342

Inhibitory effect of 2-(piperidinoethoxyphenyl)-3-(4-hydroxyphenyl)-2H-benzo (b) pyran on human endometrial hyperplasial cells mediated via suppression of Wnt/ß-catenin signaling

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ABSTRACT

Wnt/ß-catenin signaling is well known to have a prominent role in differentiation, proliferation as well as regulation of menstrual cycle in endometrium. Aberrant Wnt/ ß-catenin signaling is responsible for endometrial hyperplasia and its cancer. Endometrial hyperplasia is an overgrowth of inner layer of uterus known as endometrium Previous studies on benzopyran compound 2-(piperidinoethoxyphenyl)-3-(4-hydroxyphenyl)-2H-benzo (b) pyran (K-1) has shown the antiproliferative and apoptosis inducing activity in rat uterine hyperplasia. In our present study we have investigated the role of compound K-1 in primary culture of atypical endometrial hyperplasia. Cells were cultured and characterized by the expression of cytokeratin7, an epithelial cell marker. Results revealed that compound K-1 reduced endometrial cell viability and expression of Wnt signaling markers such as Wnt7a, fzdR6, pGsk3ß, ß-catenin cyclinD1 and c-myc. Furthermore, It was also found that compound K-1 enhanced the expression of axin and Wnt/ß-catenin signaling inhibitor Dkk-1 which caused the reduced interaction of Wnt7a and fzdR6, demonstrated by immune-precipitation. Nuclear accumulation of ß-catenin was also found to be decreased by K-1. These results suggest that compound K-1 suppressed the growth of human primary endometrial hyperplasial culture cells via discontinued Wnt/ß-catenin signaling. Thus compound K-1 may have potential as a therapeutic agent against atypical endometrial hyperplasia.

PP-343

Optimization of fermentation and downstream purification process for Coenzyme Q_{10} production using *Sporidiobolus johnsonii* mutant strain

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ABSTRACT

Coenzyme Q_0 (CoQ_{10}) is one of the new generation blockbuster nutraceuticals, which is being used extensively in supportive treatment of cardiomyopathy, cancer, neurodegenerative diseases and in combination with cholesterol lowering statin drugs that deplete the CoQ_{10} levels. CoQ_{10} functions as an electron transport agent in respiratory chain generating ATP and a potent lipid soluble antioxidant preventing lipid peroxidation [1]. Large-scale production of CoQ_{10} using chemical synthesis has several disadvantages in terms of purity, cost and selectivity. Microbial fermentation processes are widespread and score over synthetic route of CoQ_{10} production [2]. Genetic engineering efforts for CoQ_{10} production in *E. coli* are not very encouraging in terms of production yields. Hence the commercial process relies on bacterial and yeast mutant strains, which are high producers of CoQ_{10} [3]. *Sporidiobolus johnsonii*, a heterobasidiomycetes yeast strain is known to produce CoQ_{10} when cultivated under submerged conditions and there are very few reports on its bioprocess [4]. During our efforts to generate high CoQ_{10} producing mutant strains from *Sporidiobolus johnsonii*, mutant EA22 was found to produce better yield [5]. This mutant was further selected to scale up the production process. The fermentation and downstream purification process was optimized in order to get the better quality and quantity of product. The fermenter optimization was carried out with respect to media design, aeration and agitation, temperature and fed batch condition. The extraction, isolation and purification methods were optimized using chromatographic methods. The purified CoQ_{10} was characterized using analytical techniques and compared with standard compound. This poster will describe the optimized process and conditions for Coenzyme Q_{10} production using *Sporidiobolus johnsonii* mutant strain.

PP-344

Prevalence of fluorosis in primary dentition in Udaipur city, Rajasthan

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ABSTRACT

The study presents the data on prevalence of Dental fluorosis in primary dentition and finds its association with the fluoride concentration in water in Udaipur city, Rajasthan. Udaipur city was divided into five different zones namely East, West, North, South and Central zone. A total 1157 kinder garden students in the age group 3 to 5 years from 19 different schools of five zones were selected and was examined for dental fluorosis using the Dean's Fluorosis Index. A total of 1157 students with mean age group 4.06±0.84 examined for the dental fluorosis, the prevalence rate was 43.1% (n=499), with incisors being more affected 85.77% followed by canine 13.82% and molars 0.4% with $p = 0.496$ (statistically non significant). However there was a strong significant association between zones and severity of dental fluorosis with $p<0.005$. The result of this study shows that the prevalence of primary tooth fluorosis is high in the fluoride belt area of India which includes Udaipur, Rajasthan. It depicts that incisors are dominantly affected by fluorosis as compared to other primary teeth. Also primary dentition fluorosis prevalence and severity was more in the zones where the fluoride concentration of water was high.

PP-345

Ecofriendly synthesis of some biologically active heterocyclic compounds containing benzothiazole and triazine moieties

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ABSTRACT

Benzothiazole moiety constitute an important class of heterocyclic compounds possessing diverse type of biological activities viz. antibacterial ,fungicidal ,antituberculotic ,antiallergic ,anticancer etc.Triazine derivatives are also associated with broad spectrum antibacterial ,antifungal , antiviral activity against numerous viruses viz. *Rauscher viruses*, *Leukemia Moloney viruses*, *Leukemia Rhinovirus type-2,influenza virus type-2*,*Vaccinia viruses*, *Vasicular stomatitis* and *Measules viruses*. Microwave-assisted organic synthesis has attracted attention in recent years due to enhanced reaction rates, high yields, improved purity, ease of work up after the reaction and ecofriendly reaction conditions compared to the conventional methods. The present work reveals the comparative aspects (conventional and microwave) of synthesis of some heterocyclic compounds containing benzothiazole and triazine moieties and their characterization. The synthesized compounds were tested for AST (Antimicrobial Susceptibility Test) against various bacteria and fungi using standard methods.

PP-346

In vitro Detection of Antioxidant activity of *Lactobacillus* Isolates

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ABSTRACT

Lactobacilli are important member of healthy human microbiota as they are attracted a lot of attention for their potential probiotic effects. Kullisaar *et. al.,* [1] and Lin and Chang [2] have been shown that some lactobacilli possessing antioxidant activity reduce the oxidative stress during ingestion of food. In this study the antioxidant activity of three *Lactobacillus* isolates namely *Lactobacillus plantarum* CM1, *Lactobacillus rhamnosus* CM4, *Lactobacillus casei* CM6 isolated from cow milk collected from local dairies in Udaipur city, was investigated using *in vitro* methods including linolenic acid test and ferric reducing antioxidant power assay (FRAP assay). All the three *Lactobacillus* isolates namely showed demonstrable antioxidant activity. The inhibition of peroxidation of linolenic acid showed by *Lactobacillus plantarum* CM1, *Lactobacillus rhamnosus* CM4, *Lactobacillus casei* CM6 was 32.2%, 24% and 32.8% and FRAP reduction showed by them was 514.45 micromole, 463.88 micromole and 707.03 micromole respectively. These three *Lactobacillus* isolates can overcome exogenous and endogenous oxidative stresses and can play the role of potent probiotics.

PP-347

2-[piperidinoethoxyphenyl]-3-[4-hydroxyphenyl]- 2H-benzo(b)pyran interferes with non-genomic estrogen receptor signaling pathway and causes G1 phase arrest in endometrial cancer cells

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ABSTRACT

Endometrial cancer is one of the most common gynecological cancers in the western countries and its incidence has recently increased in Asian countries too. Since estrogens have been found to act as mitogens in endometrial cancers, a logical approach to the treatment of estrogen sensitive endometrial cancer is the use of anti-estrogens, or compounds that block the interaction of estrogens with their specific receptor. In a quest to design non-steroidal pure antiestrogen, 2-

[piperidinoethoxyphenyl]-3-[4-hydroxyphenyl]- 2H-benzo(b)pyran (K-1) was synthesized at Central Drug Research Institute. The compound is known to exhibit significant anti-estrogenic activity and inhibit uterine growth [1, 2]. In previous studies it was reported that compound K1 interfered with ER dependent classical and non-classical genomic pathway and cause apoptosis in endometrial cancer cells [3, 4]. The present study was aimed to explore the anti-proliferative effect of compound K-1 on ER dependent non-genomic signaling in human endometrial cancer cells. Results revealed that compound K-1 was able to interfere with GPR30 regulated-EGFR activation and subsequently decreased p-Erk, p-c-jun, c-fos, cyclin D1 and c-myc expression. Compound K-1 caused the arrest of cells in the G1 phase of the cell cycle and induced apoptosis in a concentration dependent manner as evidenced from Bax/Bcl2 ratio and effector caspase cleavage. Findings suggest that benzopyran derivative K-1 inhibits cellular proliferation via modulating ER dependent genomic and non-genomic signaling mechanisms, arrests cells at G1 phase and induces apoptosis in endometrial adenocarcinoma cells. In conclusion, compound K-1 appears to be potent therapeutic agent against endometrial cancer.

PP-348

Monoalkylation of Amines with Alcohol using Raney Nickel

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ABSTRACT

The alkylation of anilines with alcohols mediated by Raney Nickel (the first hydrogen auto-transfer reaction) was reported in 1955[1]. Since then the Hydrogen auto-transfer methodology for the alkylation of amines with alcohols has made a lot of progress especially in the last decade [2]. We decided to study Raney Nickel as a reagent for this transformation given its widespread use in industry, economical and ease of recycling.

Three grades of catalyst (W4, T4 and W7) were prepared according to the literature methods [3]. These catalysts were used in the alkylation of aniline with benzyl alcohol to check whether the method of preparation of catalyst affects the rate of reaction. The reaction was observed to be selective for mono-alkylation at 1:5 molar ratios of the aniline to benzyl alcohol in xylene at temperature range of 140-160°C. The catalysts were characterized by titration, X-ray fluorescence, particle size distribution, Scanning electron microscopy and X-ray diffraction. Characteristic differences in the size, surface and crystal properties of the catalysts were observed. The difference in the reactivity of the three grades of Raney Nickel was prominently seen with W4 giving excellent yields of the mono-alkylated product followed by W7 and T4 respectively. The difference in the reactivity of the catalyst could be attributed to the Aluminum content in the catalyst. The substrate scope, simplicity and selectivity for mono-alkylation makes this method one of the preferred Hydrogen Auto-transfer protocols for the alkylation of anilines.

PP-349

Shape and Electrostatic Similarity Analyses of Non-steroidal Anti-inflammatory Drugs (NSAIDs): Implications for Drug Repurposing

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ABSTRACT

Drug repurposing or repositioning has become a new-age mantra in view of the decreased pharmaceutical productivity in terms of new chemical entities (NCEs) introduced in the market. Non-steroidal anti-inflammatory drugs (NSAIDs) represent one of the most widely prescribed drug classes. The structural diversity of the NSAIDs makes them ideal starting points for a drug discovery program seeking totally unrelated activity.[1] In the present investigation, we generated the shape (ROCS[3]) and electrostatic (EON[3]) queries based on diverse NSAIDs. Using these queries (Figure 1), virtual screening on a set of 1447 FDA approved small molecule drugs (DrugBank)[2] was performed. The top 10 % hits were inspected visually and then compared with the original query feature-wise. This procedure was repeated for all the 20 drugs selected. All the hits were pooled together and duplicates removed. The interesting results of these shape and electrostatics similarity analyses are presented and the implications for drug repurposing are discussed.

PP-350

Study of selection strictures for biosorption with competence of activated carbon prepared from biomaterials for exclusion of heavy metals

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ABSTRACT

Heavy metals are non-biodegradable[1] and tend to accumulate in living organisms causing diseases and disorders. Conventional methods for their removal are often ineffective (especially at environmental levels), expensive and unavailable in developing countries. Biosorption is an emerging field in removal of heavy metals for its cost effectiveness, high efficiency, minimization of chemical and /or biological sludge, no additional nutrient requirements, and regeneration of biosorbent with possibility of metal recovery. It has great potentials for application in developing economies especially in India because of available profuse biodiversity as it involves the use of living or non-living biological materials for pollutants' removal from aqueous solutions and industrial effluents. Present paper has elucidated developments in the use of biosorbents with parameters for choice of metal, choice of sorbent for biosorption process, possible methods for modification of sorbents with a comparative study of biosorption potentials of activated carbon prepared by various techniques of activation for the remediation of waters and wastewaters.

PP-351

Modeling Autism: A Biology Approach

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ABSTRACT

Autism is the fastest growing developmental disorder in the world today. People with autism present with repetitive movements and with social and communication impairments. These impairments can range from mild to profound. With the rapid growth in this disorder and the great expense of caring for those with autism, it is imperative for both individuals and society that techniques be developed to model and understand autism. There is increasing evidence that those individuals diagnosed with autism present with highly diverse set of abnormalities affecting multiple systems of the body. To this date, little to no work has been done using a whole body systems biology approach to model the characteristics of this disorder. Identification and modelling of these systems might lead to new and improved treatment protocols, better diagnosis and treatment of the affected systems, which might lead to improved quality of life by themselves, and, in addition, might also help the core symptoms of autism due to the potential interconnections between the brain and nervous system with all these other systems being modeled. This paper first reviews research which shows that autism impacts many systems in the body, including the metabolic, mitochondrial, immunological, gastrointestinal and the neurological. These systems interact in complex and highly interdependent ways. Many of these disturbances have effects in most of the systems of the body. In particular, clinical evidence exists for increased oxidative stress, inflammation, and immune and mitochondrial dysfunction which can affect almost every cell in the body. Three promising research areas are discussed, hierarchical, subgroup analysis and modeling over time. This paper reviews some of the systems disturbed in autism and suggests several systems biology research areas. Autism poses a rich test bed for systems biology modeling techniques.

PP-352

New and Emerging Applications of Nanotechnology in Food Industry: A review

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ABSTRACT

The potential of nanotechnology have been recognized by many industries, and also commercial products are being manufactured. The main areas of nanotechnology application are in electronics, photonics, pharmaceuticals and cosmetics, food and finishes for surfaces and textiles. Nanoscience is defined as the study of phenomena and the manipulation of materials at the atomic, molecular and macromolecular scales, where the properties differ from those at a larger scale. [1] Recently, a lot of things have been discovered such as nanoparticulate delivery systems that play many different roles which are as transportation for carrying the functional materials to the desired site of action, nanoencapsulated food ingredients and additives. Nanotechnology can assist a wide field of food processing area. [2] The principle of nanotechnology in food processing is focusing more on food preservation and interactive foods. Nanoparticles can be incorporated into existing food to deliver nutrients, increased the absorption of nutrients by the body and also could increase product shelf life. The advantages of nanotechnology in food processing is to develop the texture of food components, encapsulate food components or additives, developing new tastes and sensations, controlling the release of flavours and increasing the bioavailability of nutritional components. On the other hand, the success of these advancements will be dependent on consumer acceptance and the exploration of regulatory issues. Unfortunately, nanotechnology application in food industry is still limited. However, the achievement of nanotechnology is beginning to give impact to the food industry, especially from food safety effect to the molecular synthesis of new products and ingredients.[3,4]

PP-353

Nanotechnology Advancements in Medicine and Dentistry

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ABSTRACT

Objective: To review Advancements of Nanotechnology in Medicine and Dentistry.

Contents: Nanotechnology is a multidisciplinary field that covers diverse array of devises derived from engineering, physics, chemistry and biology. The burgeoning new field of nanotechnology, opened up by rapid advances in science and technology creates myriad new opportunities for advancing medicine and dentistry and diseases treatment in human health care. Application of nanotechnology to medicine, physiology, dentistry imply material and devices designed to interact with the body at subcellular (molecular) scales with a high degree of specificity. This can be potentially translated into targeted cellular and tissue specific clinical application designed to achieve maximal therapeutic efficacy with minimal side effects.

Nanodentistry: is the future of dentistry in which every procedures will be performed using equipments and devices based on nanotechnology. All diagnosis and treatment will be given using nano particles which are less than 100nm in size and nano robots using a combination of nano medicine in biotechnology, it will become possible to revolutionise various applications examples: restoration, dentin hypersensitivity and agents of drug delivery etc. Nano particles are known to have properties like enhance resistance to heat, solvents and abrasions. Prospects are bright for aesthetic dentistry due to their small size and light absorption and transparency. Dental nano robots will be used for analgesia, plaque control agent delivery and play a major role in orthodontic therapy. This poster discuss the future of medicine and dentistry with the applied aspects of nano technology.

PP-354

Formation of novel coordination polymers from zincate dianion bearing alkanesulfonate groups in the structural frameworks

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ABSTRACT

The synthesis of a few novel coordination polymers, $[Zn(OS(O)_2Me)_2(H_2O)_2]_n$ (**1**), $[Zn(OS(O)_2Et)_2(H_2O)_4]_n$ (**2**) and $[Zn(H_2O)_6(OS(O)_2n\text{-}Pr)_2]_n$ (**3**), $[Zn(4,4'\text{-bpy})(H_2O)_4(OS(O)_2Me)_2]_n$ (**4**) and $[Zn(4,4'\text{-bpy})(H_2O)_4(OS(O)_2Et)_2]_n$ **(5)** has been achieved by reacting $[Zn(OS(O)_2R)_4]^{2-}$ (R = Me, Et, *n*-Pr), isolated by the reaction of anhydrous zinc acetate with dialkylsulfites, $(RO)_2S{=}O$ (R = Me, Et, n-Pr) in the presence of tetra alkyl ammonium iodide, with water and 4,4'-bipyridine under ambient conditions. The method involves *in situ* generation of the corresponding alkanesulfonate moieties via sulfur centered Arbuzov type rearrangement in dialkylsulfites[1]. X-Ray crystal structure analysis reveal a rich diversity of two-and three-dimensional structural motifs in which the sulfonate groups act as weakly coordinating ambidentate ligands with affinity toward H-bond interactions. Preliminary studies on the reactivity behavior of **1** and **2** with 4,4'-bipyridyl in dry methanol have afforded isostructural cationic coordination complexes **4** and **5**. The structure of **4** [figure (a)] and (b)] features a three-dimensional motif as a result of extensive H-bonding and reveals intercalation of anion in between the cationic layers.

PP-355

Organocatalytic Asymmetric Synthesis of 1,2,4-Trisubstituted Azetidines By Reductive Cyclization of Aza-Michael Adducts of Enones

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ABSTRACT

Over the years, functionalized aza-heterocycles, which are at the heart of many essential pharmaceuticals and physiologically active natural products, have attracted the attention of organic chemists in order to develop novel, synthetically useful, and elegant methodologies for the synthesis of such type of compounds as targets for design of new drugs and important intermediates in organic synthesis. Amongst chiral nitrogen heterocycles, azetidines[1,2] have received much attention during the last decade because of their utilization as ligands[3] and their biological and pharmaceutical activities.[4,5] Recently, G. Bartoli and P. Melchiorre have developed primary amine salt catalyst **A**[6] for both iminium ion catalysis and asymmetric counteranion-directed catalysis (ACDC) phenomenon,for the highly enantioselective conjugate addition of a series of different nucleophiles[7] (-C, -S, -O centered nucleophiles) to enones.[8] In our endeavors to synthesize enantiopure azetidines, we advanced this organocatalytic activation strategy to document an operationally trivial procedure for the aza-michael addition of of *N*-arylphosphoramidates **1** to a,ß-unsaturated ketones **2** catalyzed by the chiral salt **A** to give aza-Michael adducts **3** followed by the intramolecular reductive cyclization via (*R*)-Alpine borane to give 1,2,4-trisubstituted azetidines **4** (in 67-93% yield with 85-95% diasteroselectivity and 78-96% enantioselectivity) in a one-pot procedure as outlined in Scheme 1. To the best of our knowledge, primary amine salt **A** has not been used for the conjugate addition of nitrogen nucleophiles to enones till date and herein we report the first organocatalytic addition of phosphoramidates (a weak nitrogen containing nucleophile) to enones ultimately leading to enantiopure azetidines **4**.

PP-356

Chemotherapeutic potential of 2-[piperidinoethoxyphenyl]-3-phenyl-2H-benzo(b)pyran in ER- negative breast cancer cells : action via prevention of EGFR signalling

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ABSTRACT

Inhibition of epidermal growth factor receptor (EGFR) signaling is considered to be a promising treatment strategy for estrogen receptor (ER)-negative breast tumors. We have investigated here the anti-breast cancer properties of a novel anti-proliferative benzopyran compound namely, 2-[piperidinoethoxyphenyl]-3-phenyl-2H-benzo(b)pyran (CDRI-85/287) in ER-

negative and EGFR- over-expressing breast cancer cells. The benzopyran compound selectively inhibited the EGF-induced growth of MDA-MB231 cells. The compound significantly reduced tumor growth in xenograft of MDA-MB231 cells in nude mice. The compound displayed better binding affinity than EGFR inhibitor AG1478 as demonstrated by molecular docking studies. CDRI-85/287 significantly inhibited the activation of EGFR and downstream effectors MEK/ Erk and PI-3-K/Akt. Inhibition of MEK/Erk pathway led to subsequent inhibition of AP-1 promoter activity resulting in decreased expression of PCNA, c-fos and c-jun. Inhibition of Akt led to dephosphorylation of downstream effectors FOXO and NF?B leading to increased expression of p27. Decreased p27 led to decreased expression of cyclin D1 and decreased phosphorylation of Rb which would result in prevention of transcription of E2F- dependent genes involved in cell cycle progression from G1/S phase evidenced by flow cytometry. The compound induced apoptosis via mitochondrial pathway and it also inhibited EGF-induced invasion of MDA-MB231 cells as evidenced by decreased activity of MMP-9 and expression of CTGF. Results suggested that benzopyran compound CDRI-85/287 could constitute a powerful new chemotherapeutic agent against ER-negative and EGFR over-expressing breast tumours.

PP-357

Synthesis of an efficient, recyclable and eco-friendly volcanic ash supported solid acid catalyst OR Volcanic ash supported solid acid: An efficient, reusable and eco-friendly catalyst

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ABSTRACT

New environmental legislation calls for the reduction of waste production and use of more environmental friendly alternative catalysts attract us to develop some activation techniques to make an innovative use of volcanic ash, a solid waste product. Volcanic ash is a silica enriched material having higher degree of fineness, larger surface area and more acting faces, which illustrates higher activity. These features of volcanic ash make it suitable to be used as a catalytic support for several industrially important organic transformations. For this purpose, volcanic ash was collected from a chemical industry. Different activation methods such as mechanical activation by ball milling and hand milling, thermal activation by calcination at temperature ranging from 100-1000°C and chemical activation by treatment with conc. sulphuric acid were applied to optimize the conditions for maximum yield of desired product. The physio-chemical properties of the prepared catalyst (AVAC) were determined by using FT-IR, SEM, AAS etc. While the catalytic activity was evaluated by the liquid phase esterification reaction of 1-butanol and acetic acid under optimized conditions, resulting into 1-butyl acetate, used in paints, perfume industries. The catalyst can be regenerated and reused up to three cycles with similar efficiency as in first run. Our present work proposed that by means of appropriate treatment, volcanic ash can be converted into potential solid acid catalyst in order to replace conventional, environmental hazardous liquid acids.

PP-358

Perlite supported heterogeneous base catalyst : Characterization and application

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ABSTRACT

Modern environmental legislation calls for reduction of waste and waste production. Use of environmental friendly alternative catalysts attracts us to develop some activation technique to make an innovative use of perlite, a siliceous waste material. Perlite is silica enriched, inert and non toxic material having small grain size, light-weight, less dense particles and high surface area which represent high surface activity of perlite. Due to these features perlite can be used as a good solid support material for preparation of industrially important heterogeneous catalyst synthesis. Heterogeneous catalyst is formed by using different activation techniques such as mechanical activation by ball milling and hand milling, thermal activation by calcination at temperature ranging from 100-1000°C and chemical activation by treatment with different bases. Physiochemical properties of prepared catalyst (BEPC) were determined by using FTIR, SEM, XRD, TEM while the catalytic activity was measured by liquid phase, solvent free, single step condensation of benzaldehyde with cyclohexanone giving higher conversion desired product a, a '-dibenzylidenecyclohexanone. The catalyst can be reused and regenerated upto 4 reaction cycles with similar efficiency as in first run. The application of perlite to synthesize a solid base catalyst finds a noble way to utilize this abundant waste material.

PP-359

CRYSTAL STRUCTURE, LIGATION BEHAVIOUR AND DFT STUDIES OF 5-HYDROSELENO SALICYLALCOHOL (L^1)

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ABSTRACT

Selenium bearing 5-Hydrolseleno salicylalcohol ($\mathbf{L^1}$) was prepared by the interaction of disodiumselenide, and 5-chloro salicylaldehyde. The ligation reaction of $\mathbf{L^1}$ was also examined using $HgCl_2$ **(1)**. $\mathbf{L^1}$ and complex **1** have been characterized by elemental analysis, TEM, IR, ^1H, ^{13}C NMR and ESI mass spectra, X-ray analysis and DFT analysis.

PP-360

Lead exposure and histopathological alterations in postnatal development of testis

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ABSTRACT

The magnitude of occupational and environmental reproductive and developmental health risks in modern society is still being studied. Scientific, epidemiological, and toxicological data concerning the reproductive and developmental health risks have been determined for some chemicals. Despite the scientific studies carried out over the years, on the toxic effects of lead on development of organism, still there are uncertainties over the reproductive effects of different levels of lead exposure. It is undeniable that good quality semen is essential for reproductive success. This quality appears to have been directly affected by multiple uses of heavy metals. In the present investigation the effects of lead acetate was studied on the postnatal (7^{th} day) development of testis. Two dose levels (8mg/kg/BW and 16mg/kg/BW) were selected and given from the 10^{th} day of gestation and throughout lactation. Microscopic examination revealed that lead induced apparent damage and reduction in the number of seminiferous tubules and primordial germ cells. Daily exposure of lead acetate during pregnancy and lactation causes a significant decrease in the developing germ cells and reduction in the germinal epithelium. Oral exposure of lead acetate changed the arrangement and shape of spermatogonia cells and reduced the number of Sertoli cells. It also diminished the development of Leydig cells. We can conclude from our findings that lead can cause histopathological alterations in developing testis of Swiss albino mice. Exposure of lead caused significant alteration in development of male gonads at different dose level of lead acetate. The histopathological modification in the basic precursor of gonads during the postnatal development causes reduced fertility in adulthood.

PP-361

Synthesis and Biological Evaluation of Novel Isoxazole Derivatives as prospective Anti-inflammatory Agents

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ABSTRACT

An effort to discover an ultimate magic bullet to treat inflammation continues to be an important drug design challenge but, the therapeutic effectiveness of these agents has been limited by cardiovascular, renal, hepatic and gastrointestinal side effects. Due to this, the development of novel, selective, potent and safe agents, effective against cyclo-oxygenase enzyme remains in high priority in medicinal chemistry research. The present study has sought to undertake the structural modifications of isoxazole ring skeleton to produce synthetic analogs in which C-2 of isoxazole ring is substituted with a number of different heterocyclic scaffolds. Synthans, such as oxoketenedithioacetals are known in the literature to offer unprecedented opportunity

to a chemist in the synthesis of a wide variety of difficultly accessible heterocyclic compounds. It has been demonstrated that oxoketenedithioacetals react smoothly with bidentate nucleophile like hydroxylamine hydrochloride, and provide a very convenient synthetic entry to the isoxazole nucleus. This methodology when applied on deoxybenzoin (1) with CS_2 and CH_3I afford the corresponding oxoketenedithioacetal derivative (2). Treatment of 2 in the subsequent step with hydroxy lamine hydrochloride generated the corresponding isoxazole derivative 3 whose reaction with $ClSO_3H$ followed by NH_3 resulted 5. The lactim thioether of 5 reacted with a variety of bioactive primary and secondary amines to afford the products 6-21 respectively as shown in Scheme 1. The microanalysis, IR, ^{1}HNMR and MS data of 6-21 were found to be consistent to the structures assigned to the molecules. The synthesized compounds have been found to show promising anti-inflammatory activity in wistar rats. Furthermore, except 19 none of the synthesized molecules had shown Lipinski violation.

PP-362

Computational Studies on Glycogen Synthase Kinase-3ß (GSK-3ß): Targeting the Allosteric Sites

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ABSTRACT

Glycogen synthase kinase-3ß (GSK-3ß) is a fascinating enzyme with diverse number of actions in intracellular signalling systems. It plays a key role in type II diabetes, Alzheimer's disease and Bipolar disorder (Castro *et al)*. In comparison to the active site of the enzyme, the allosteric site presents an opportunity for development of selective inhibitors (Valle *et al*). In addition, the structural adaptability of the allosteric site could afford increased flexibility in drug design, which can be of crucial importance in satisfying pharmacokinetic and toxicological criteria. This leads to the hypothesis that inhibition of GSK-3ß may have therapeutic benefit in treating these disorders. In an attempt to identify new ligands for GSK-3ß, virtual screening (VS) model was developed based on two-dimensional (2D) pharmacophore similarity, physicochemical scalar descriptors, an ADME/Tox filter, and three-dimensional (3D) pharmacophore searches. Molecular docking studies were performed for diverse compounds on druggable binding sites of the enzyme (Martinez *et al)*. Further computational studies were carried out using data from resources of authentic agencies such as Spec and Zinc database. Target specific computational models were developed which can identify the ligands that can selectively modulate GSK-3ß at allosteric sites; using these, commercial databases were screened with GOLD and Discovery Studio from which few templates were identified. These templates would serve as a starting point for further development of GSK-3ß inhibitors which can be useful for new candidate design.

PP-363

X-ray crystallographic study and DFT calculations of 3,4,6,7-tetrahydro-3,3,6,6-tetramethyl-2H xanthenes 1,8(5H,9H) dione

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ABSTRACT

In the present study xanthene dione, a coumarin derivative, was synthesized and studied by X-ray crystallography and theoretical methods. Xanthene dione is a biologically active molecule that shows good antibacterial and antifungal properties and is an optically active compound. The molecule crystallizes in triclinic crystal system with P-1 space group. Density functional theory (DFT) calculations were performed at Becke's three-parameter functional and Lee–Yang–Parr functional (B-3LYP) level of calculation and the 6-31G++ basis set was used for ground state geometry optimization. The *xyz* coordinates obtained via X-ray crystallography have been taken for the geometry optimization in DFT. A close comparison of the selected bond lengths and bond angles of the crystal structure and theoretically optimized structure by DFT have shown only marginal difference. The DFT study of electron surface potential (ESP), showed a large intramolecular charge transfer efficiency of the molecule indicating optical active of xanthene dione.

PP-364

Novel point mutations in the antifolate drug resistance marker genes among *Plasmodium vivax* isolates exhibiting severe manifestations

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ABSTRACT

Plasmodium vivax is one of the predominant species of the human malaria parasite present in the Indian subcontinent. There have been recent reports on Chloroquine resistance and severe manifestations shown by Plasmodium vivax from different regions of the world including India. This study focuses on Bikaner, India where during the last few years there have been continuous reports of severe manifestations by both P.falciparum and P.vivax. Kochar et al. [1]. Chloroquine and Sulfadoxine-Pyrimethamine have a widespread use for treating malaria in this region, but the resistance profiles of these drugs are not available. We report here the profile of mutations in marker genes associated with Chloroquine and antifolate drug resistance among the P.vivax parasites obtained from patients with severe and non-severe manifestations. Most isolates showed the wild type alleles for both of these markers ($P<0.0005$). The frequency of PvDHFR-PvDHPS two locus mutations was higher among the patients showing severe manifestations than patients with uncomplicated malaria ($P<0.003$). Novel mutations in PvDHFR and PvDHPS were observed only in the parasite population from patients exhibiting severe complications. Preliminary homology modeling and molecular docking studies predicted that these mutations apparently do not have any effect on binding of the drug molecule to the enzyme. However, the presence of novel mutations in the PvDHPS gene indicate polymorphic nature of this molecule which is in contrast to available published information. Garg et al. [2]. We have also studied the expression pattern of these genes in severe malaria cases. The microarray expression data showed any one of the genes; Pvcrt or Pvmdr-1 to be upregulated. Recent reports have also suggested an increased expression of the chloroquine resistance marker genes in severe vivax malaria. These findings supports to further explore potential of *these genes as* molecular markers of severe disease in *P. vivax*.

PP-365

Characterization and Production of pectinolytic enzymes by Xanthomonas axonopodis citri isolated from various sources

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ABSTRACT

Xanthomonas are yellow pigmented motile, aerobic rods mostly pathogenic to cultivated and wild lants. Species of Xanthomonas causes some of the most serious diseases in plants. Seventy eight Xanthomonas axonopodis citri (Xac) strains were isolated from citrus rinds, leaves and stem. Xac produces extracellular cell wall degrading enzyme that degrade the pectic layers of plant cell wall and provide entry in the host plants. Pectinesterase (PE), Polygalacturonic acid trans-eliminase ((PATE), Pectin methyl esterases (PME), Pectin lyases(PL) and Pectate lyases(PAL) are produced on pectin or pectic acid based medium by all Xac strains screened. Pectinesterase production was found in the culture containing pectin as the substrate rather than polygalacturonic acid or glucose. PE, PAL and PME activity was found in higher concentration than PL and PATE Xac isolated from leaves. Xac isolated from stem showed only PE and PATE activity. PME, PL and PATE enzyme were synthesized by Xac isolated from citrus rind

PP-366

Studies on acetoin biosynthesis in Bacillus Subtilis

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ABSTRACT

Acetoin is hydroxyl-keto compound that is used as a secondary carbon source in some organisms like *Bacillus subtilis* during sporulation. To understand the bottleneck for acetoin biosynthesis; variation of acetoin biosynthetic operon copy no and expressed a heterologous pathway (*Zymomonas mobilis* pyruvate decarboxylase) was performed. Experiments by varying initial glucose concentration and addition of pyruvate at selective growth phase suggest that pyruvate (direct substrate) concentration is more critical then initial carbon source concentration for acetoin accumulation. By comparing the data between 168alsSD and 168alsR-, it is clear that acetoin biosynthesis pathway is important for efficient utilization of pyruvate and it only have effect during stationary phase of growth. As expected, expression of ZmPDC causes redox imbalance and hence flux shifts towards acetoin to 2, 3 butanediol. That shows another important function of *alsSD* operon for maintaining NAD/H+ balance in *Bacillus subtilis*. The study revealed that pyruvate is an important metabolite to study for development of strategy for accumulation of secondary metabolites like acetoin and 2, 3 Butanediol.

PP-367

Performance Analysis of PCA & DWT for Biomedical Image fusion

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ABSTRACT

Image Fusion is the process of combining images from different sources to obtain a single composite image with extended and enhanced image content, superior to the base images. The Image fusing techniques aim at fusing such images to improve the perceptibility or information content of a scene. Medical imaging fusion plays an important role in the diagnosis and treatment of patients with cancer who are receiving radiation therapy.

In this paper, Biomedical Image Fusion by PCA & DWT will be developed with Matlab as the working environment and tested with simulated images. These images will then be enhanced and fused using the algorithms developed and the quality assessed with visual perception and metrics calculated such as entropy ,PSNR, Quality Index, correlation coefficient etc. The performances of the two methods are then compared and results obtained are presented. It has been concluded that image fusion using wavelets transform showed better performance by visual perception and in metrics, than principal components analysis.

PP-368

KINETICS AND MECHANISM OF L-HISTIDINE BY MANGANESE (III) IN PYROPHOSPHARTE MEDIUM

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ABSTRACT

Kinetics of oxidation of L-Histidine by Manganese (III) has been studied in pyrophosphate medium. The reaction shows first order dependence on $Mn(III)Py^{3}$, L-Histidine & fractional order with respect to $[H^{+}]$. The rate of oxidation decreases dielectric constant of solvent suggesting ion-dipole interaction. Addition of $MnSO^{4}$ & $Na^{2}P^{4}O^{7}$ shows retarding effect on rate of reaction. Activation parameters have been evaluated. A mechanism consistent with experimental observations has been proposed.

PP-369

Peganine Hydrochloride isolated from Peganum harmala seeds Protects gastric mucosa in rats

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ABSTRACT

Peganum harmala Linn, commonly known as 'harmal' belonging to the family Zygophyllaceae, is one of the most important medicinal plants of India. [1] Its different parts are used in traditional systems of medicine for the treatment of variety of human ailments. [2] In continuation of our drug discovery program, we explored the protection of gastric mucosa in rats using standard protocol, [3] by Peganine hydrochloride which was isolated from the seeds of Peganum harmala. Peganine hydrochloride was found to possess anti-ulcerogenic activity which might be due to its anti-secretory activity and subsequent strengthening of the defensive mechanism.

PP-370

Synthesis, characterization and biological evaluation of some pyrazoline derivatives

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ABSTRACT

A new series of pyrazoline derivatives have been synthesized from the new class of conventional methodology. Pyrazolines are a variety of heterocyclic compounds with five membered ring There are number of molecules with five membered rings containing 'N' as a hetero atom but pyrazolines are proven in several biological aspects including antimicrobial, anti tubercular, antiviral and insecticidal etc., the synthesized entities were screened for their antitubercular activity against *M.tuberculosis H37Rv* and also antimicrobial activity against various class of microorganisms. The final results revealed that most of the tested heterocyclic moieties showed promising activity against all the microorganisms employed. The synthesized heterocyclic derivatives were characterized by IR, ^{1}H NMR, ^{13}C NMR and elemental analyses studies.

PP-371

TBAB-catalyzed reactions for efficient synthesis of indole derivatives in aqueous micellar media : A convergent approach

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ABSTRACT

This century has witnessed an increasing interest in the development of economically simple and environmentally safe methods in synthetic organic chemistry. In this regard, green chemistry approaches offer significant potential to reduce by-products, waste produced and energy costs as also in the development of new methodologies for previously unobtainable materials.

Recently, aqueous environment has attracted much attention in organic synthesis. The development of organic reactions in water has become highly desirable to meet environmental considerations. The unique properties of water like high dielectric constant and cohesive energy density showed an extra ordinary effect on reaction rates. Moreover, its cost-effectiveness, high abundance, non-inflammability and non-toxic nature has increased its applicability. Surfactants have attracted significant attention because of their high catalytic activity and benign character in the context of green chemistry, which provides a way for alternative synthetic routes in an aqueous medium. Heterocycles occupy a prominent position as nature has chosen several of these to carry out various physiological and biochemical functions in living cells. Amongst the various heterocycles, indole and its derivatives possess interesting biological activities and are widely used as a precursor for many natural products.

With an aim to develop more efficient and mild synthetic process for developing new selective and environmentally benign methodologies for the synthes is of bioactive heterocycles, we here in, report for the first time, a new greener procedure for the synthesis of indole derivatives, *viz.*, 3'*H*-spiro[indole-3,2'-[1,3]benzothiazole]-2(1*H*)-ones, 6*H*-indolo[2,3-b]quinoxalines and 3-(2-hydroxy -phenylimino)-1,3-dihydro-indol-2-ones by the reactions of indole-2,3-diones with 1,2-difunctionalized benzenes *viz.* o-aminothiophenol, *o*-phenylenediamine and o-aminophenol, respectively in aqueous micellar medium using tetrabutylammonium bromide (TBAB), as a surfactant while reaction does not take place with 1,2-dihydroxy benzene under the optimized conditions. The chemical structure of the synthesized compounds were established on the basis of their analytical as well as spectral (IR, ^{1}H NMR, ^{13}C NMR and Mass) studies.

PP-372

Study of Cledendron Plumidis Plant Extract on Intestinal Worms of Commertial Birds with Special Reference to Inorganic Ions in Blood Serum

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ABSTRACT

Cleredendron phlumidis is a flowering shrub or small tree characterized by a foetid smell. Itsleaves are vermifuge and its juice is used to destroy worms. The present study deals with the curative impact of water extract of *cleredendron plumidis on intestinal worms of commertial birds with respect to inorganic ions in blood serum.*, ,chickens are divided in to four groups.Cage 1 is used as control in which chickens were maintained as it is with regular food supply & necessary maintenance in case No. 2 chickens were given to the faces of pig containing intestinal worm cysts through food material. In cage No. 3 the induced chicken were also treated with the water extract of *Cleredendron Plumidis.* In cage no 4 chickens were treated only with the water extract of *Clerendendron phlumidis.*

KEY WORDS- cledendron plumidis, intestinal worms , commertial birds inorganic ions

PP-373

Band structure and electronic properties of transition metal chalcogenide WTe_2

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ABSTRACT

Layered compounds of the transition-metal dichalcogenides (TMDCs) of group VI-B have been studied since last four decades [1]. They are widely used in photovoltaic and opto-electronic devices [2], as their band gaps are of the order of the solar spectrum. WTe2 which has sufficient technological applications in photo electrochemical cells, semiconductors, batteries, catalysts and solid lubricants at high temperatures still has a very less number of theoretical and experimental studies for electronic structure calculations. It crystallizes into a trigonal prismatic structure (2H-structure) in which a sheet of metal atoms is sandwiched between two sheets of chalcogens. In this paper, we report the first ever studies of the electronic properties of 2H-WTe2 by full potential linearised augmented plane-wave [3] method. To obtain self-consistency, we have undertaken relativistic calculations using the non-empirical DFT-GGA suggested by Wu and Cohen [4].The band structure calculations show that 2H-WTe2 is an indirect-gap semiconductor with the valence band maximum at the G point and the conduction band minimum about midway between the GK direction of the hexagonal Brillouin zone. The energy bands show strong covalent intra-layer bonds, whereas the sandwiches are separated by van der Waals gap.

PP-374
Synthesis, characterization and photophysical properties of novel *meso*-triazole linked porphyrin-coumarin conjugates

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ABSTRACT
Porphyrins are an important class of heterocycles which play very essential roles in diverse biological processes. Among various natural pigments, these tetrapyrrole macrocycles are known to exhibit high absorption coefficient and rapid excited-state energy transfer characteristics [1]. In addition, heterocycles containing triazole tethered coumarin systems have demonstrated outstanding optical properties [2] and are found useful as energy transfer donors in dendrimers [3-6]. By considering unique photochemical properties of these two classes of molecules, it was contemplated to construct new *meso*-triazole linked porphyrin-coumarin conjugates by combining the porphyrin, triazole and coumarin moieties in a single molecular frame work. Such hybrid molecules may prove useful for the development of new molecular materials with enhanced photochemical and electrochemical properties.

P-375
Biocompatible silver nanoparticles from marine isolate Streptomyces parvulus and biogenic properties

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ABSTRACT
Protein encapsulated synthesis of silver nanoparticles by an isolated marine actinomycetes strain has been investigated. The selective isolate is gram-positive in nature and belongs to Type-1 class of actinomycetes. Chemotaxonomic evaluation of cell wall composition suggested that this strain belongs to Streptomyces parvulus which was further confirmed based on 16S rRNA phylogenetic analysis. Spherical shaped monodispersive and crystalline silver nanoparticles production was observed within 24 h incubation time. The biosynthesized particles showed single Surface Plasmon Resonance (SPR) at 421 nm. TEM studies revealed that the produced silver nanoparticles are spherical in shape. The particle size distribution revealed the size of produced particles ranges from 1.66 – 11.68 nm with a mean size of 2.1 nm. The synthesized silver nanoparticles exhibited stretching vibrations of primary and secondary amines along with C-H and C-N indicating the metabolically produced proteins involvement in size regulation of reduced silver nanoparticles. An average negative zeta potential value of 81.5 mV with an electrophoretic mobility of 0.000628 cm^2/Vs was observed with poly-dispersive index ratio of 0.96. The biosynthesized nanoparticles revealed antimicrobial property against gram negative as well as gram positive bacterial strains with variation in MIC values as well as antioxidant activity. This study suggested that the isolated marine Streptomyces parvulus SSNP11 has potential to produce silver nanoparticles and can be exploited for bulk production of reproducible, mono-dispersive, spherical and 2.1 nm mean size silver nanoparticles using green approach.

PP-376
Effect of Physical Factors on Antimicrobial Potency of *Polyalthia longifolia* Leaf Extract

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ABSTRACT
Antimicrobial activity of plant extracts depends on the chemical nature of compounds present in them. Various physical factors such as pH, temperature, exposure to sunlight may bring about a change in chemical nature of these compounds thereby affecting the antimicrobial property of the extract. Effect of pH, temperature, sunlight etc. on minimum inhibitory concentration (MIC) of leaf extract of *Polyalthia longifolia* against *Aspergillus fumigatus, Alternaria solani, Escherichia coli and Salmonella typhi* has been studied to check its stability. Effect of heat, sunlight and pH on the viability of extracts was assayed according to the method suggested by Rath *et al*., Wang and Ke-Qiang and Shahi *et al.* respectively.. Dry heat up to 80°C did not affect the activity of extract whereas wet heat treated extract showed very slight reduction in activity at 100°C. No change in activity was observed due to exposure to direct sunlight for 15 h and 30 h . At neutral pH which is the normal pH of extract, no change in activity was observed. At pH 4 and pH 9 extract activity was reduced but reduction was slightly more at alkaline pH as compared to acidic pH.

PP-377

Synthesis of New Oxazines/Thiazines-Heteroaromatic Conjugates *via* Multicomponent reaction

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ABSTRACT

Multi-component reactions (MCRs) have been emerged as an extremely powerful tool in combinatorial chemistry and drug discovery, since it offers significant advantages over conventional linear step syntheses, in terms to improve classical organic reactions, promote new reactions and develop straightforward synthetic routes for bioactive heterocycles and other complex molecules.[1]

Most of the natural products and drugs contain heterocyclic cores in their structures. Some of the drug analogues/hybrid molecules contains more than two heterocyclic rings and shows interesting biological activities, viz., antimicrobial, antimalarial, anti-inflammatory, antitumor, anti-HIV, anti-cancer and anti-parasitic. Thiazine core is an important in various dyes and tranquilizers. 1,3-oxazine derivatives are potent antitumor agents. We envisioned that synthesis of various oxazines/thiazine-heterocyclic conjugates that leads to the new hybrid compounds could be the good precursor for novel hypoxia targeted compounds for cancer therapeutics.[2]

We have synthesized new 1,3-Oxazines as well as Thiazines by multi-component Biginelli-type condensation reaction[3] of alkyne, urea/thiourea and heterocyclic aldehydes provide a series of 2-amino-4*H*-1,3-oxazines and 2-amino-4*H*-1,3-thiazines in good to excellent yields (**Scheme 1**).

PP-378

Screening of Sweet Shop Effluents for Isolation of Extracellular Polysaccharide Producing Bacteria

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ABSTRACT

The biochemical diversity of the microbial kingdom is reflected in the varied applications of microorganisms. Microbial exopolysaccharides (EPS) are the primary or secondary metabolites produced by a variety of microorganisms. Microbial polysaccharides are good substitutes of gums obtained from plants and marine algae. They are eco-friendly in nature and susceptible to natural biodegradation causing little damage to environment and thus diminishing pollution. Guezennec [1], Silvia and Crispin [2] reveals the reports of isolation of exopolysaccharides secreting bacteria from milk products, fermented food products, psycrophilic regions, deep sea hydrothermal vents, soil. Sweet manufacturing process use milk, milk products and sugar which generate effluents rich in organic and inorganic nature that harbor as a habitat for EPS producing bacteria. The present study reports the isolation of EPS producing bacterial strain from sweet manufacturing unit effluent which were identified as *Agrobacterium* species based on the morphological, biochemical, cultural characteristics. The bacterium was creamish yellow in colour with convex and circular colony morphology. They were Gram negative rods appearing as single rods or rods in pair and were negative for the presence of endospores. Biochemical characters of the isolate were positive for catalase, oxidase, lactose, mannitol, sucrose etc. The nucleotide homology and phylogenetic analysis based on 16s rRNA sequences confirmed that the bacterium represents *Agrobacterium tumefaciens.* The bacterium produced both floating and precipitating EPS in a medium containing sucrose as the carbon source. The polysaccharides were lyophilized and their dry weights were 6gms/litre and 30 gms/litre respectively.

PP-379

Effect of different Inhibitors on Calcium Phosphate and Calcium Oxalate Mineralization potential of simulated Urine at different conditions

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ABSTRACT

This experiment was planned to evaluate the influence of inhibitors on calcarious stone formation (Pathari) in the conditions when spontaneous precipitation can occur. Here the effect of magnesium, citric acid, pyrophosphate, Gylcosaminoglycans(GAGs) on the calcification process in simulated urine was examined with two variables i.e. Concentration of Inhibitors and pH.

Having this proved from our previous experiments,(1) relatively greater and more important role of inhibitors than stone promoters in crystal clotting process, a experiment was planned to ascertain the behaviour of some known inhibitors in relation to their conc^{n}&pH. Simulated Urine was selected for this purpose to get results comparable with natural urine. The simulated urine was prepared by mixing fourteen ingredients in suitable proportions.(2). The levels of pH selected were between 5.0 – 7.5 because over 90% of the stone formers in Rajasthani population fell in this group.

The different concentration of inhibitors was decided keeping in mind hypo and hyper excretion of these substances .In the control system, the calcium precipitation was found to increase with increasing pH (5.0 to 7.5). The calcium in soluble fraction was 69.6, 66.6, 39.6 and 16.7% respectively. All the substances tested showed inhibitory acticity in acidic medium. The apparent effect of these inhibitors showed different trends but do confirm their participation as inhibitors. To get the actual idea about theireffects in relation to pH, concentration and on their interaction the statistical exercise of analysis of variance (ANOVA) was undertaken.

The results of analysis give the lucid idea that inhibitors have a significant interaction thereby indicating that these are not acting independently and that both pH and conc^{n} of these inhibitors also significantly affected the process of Calcium Oxalate and Calcium Phopsphate stone formation. It is also evident that the effect of individual inhibitor is not simple addictive one, rather it is a combined venture with a joint proportionate influence.

In conclusion, it can be stated that Inhibitory behaviour is selective and is concentration and pH related.

PP-380

Structural and magnetic properties of nanosized $CoCrFeO_4$ prepared by solution combustion method

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ABSTRACT

Spinel ferrites are important class of magnetic materials which have a growing interest for use in understanding the basic electronic and magnetic properties and also for technological applications. Chromites are known to be frustrated magnetic systems because of the exchange interaction between Cr ions at the B-sites and so it is interesting to study the magnetic properties on replacement of Cr with Fe which is expected to modify the frustration in the system. Oxide materials can be prepared by various techniques of which the solution combustion method is one through which highly pure, crystalline and homogeneous material can be prepared with high yield. Nanosized CoCrFeO4 sample reported in this study has been prepared by using analytical grade metal nitrates and citric acid. The metal nitrate to citric acid ratio was kept at 1:1. X-ray diffractometry confirms formation of a single spinel phase with lattice parameter 8.401Å and average crystalline size of 4nm. RT Mössbauer spectra of the sample show superparamagnetic doublets while a non saturating hysteresis curve with coercivity of 400Oe is obtained at RT. To understand more about the magnetic state present in the system, low temperature magnetic measurements are carried out. Magnetic irreversibility is evident since the zero field cooling (ZFC) and field cooling (FC) curves shows bifurcation up to RT. Blocking temperature of 140K us obtained from ZFC measurements. The high magnetic frustration present in the present sample is evident in the open hysteresis loop obtained at 20 K after ZFC. At 20K, the coercivity increases to 1.8kOe and interestingly there is also a loop shift after ZFC cooling of about 175Oe indicative of the magnetic frustration in the sample which thus is also promising for use as a multiferroic material.

PP-381

Characterization of *Brugia malayi* Guanylate kinase : a putative drug target

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ABSTRACT

Nucleotide metabolism is a key pathway in life cycle of any organism and its enzymes lead to the production of nucleotide triphosphates (NTPs) which are DNA and RNA precursors. The de novo pathway involving the synthesis of purine nucleotides is present in host while filarial parasites possess salvage pathway for purine synthesis. Guanylate kinase (ATP:GMP phosphotransferase , guanosine monophosphate kinase, EC 2.7.4.8) belongs to nucleoside monophosphate kinase superfamily and is critical for the synthesis of GTP/dGTP since it catalyses reversible phosphorylation of GMP/ dGMP to its diphosphate form GDP/dGDP. It's inhibition will modulate the synthesis of nucleotides, which are indispensable for any organism. In addition to being a critical enzyme in the biosynthesis of GTP and dGTP, Guanylate kinase functions in the recovery of cGMP and is ,therefore, thought to regulate the supply of guanine nucleotides to signal transduction pathway components.

In the present study, Guanylate kinase of human filarial parasite *Brugia malayi* (BmGK) was cloned in pET28a expression vector , overexpressed in E.coli BL21(DE3) host cells and protein was purified by Ni-NTA affinity chromatography. Kinetic studies conducted on BmGK showed maximum activity at pH 7.5 and 37^{o}C. Filarial enzyme differs from its host enzyme in its kinetic parameters. Km value calculated for both substrates GMP and ATP were 30µM and 110 µM respectively. GMP was utilised as the preferred substrate followed by dGMP showing 75-80% activity. Similarly, among different NTPs tested, ATP was the preferred phosphate donar followed by dATP.

PP-382

A FACILE SYNTHESIS, CHARACTERIZATION AND STUDY OF BIOLOGICAL ACTIVITY OF SOME NOVEL SERIES OF 3-SUBSTITUED-4-(4/5-SUBTITUTED-3-INDOLYLIDENE)AMINO-5-MERCAPTO-1,2,4-TRIAZOLES AND THEIR MANNICH BASES .

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ABSTRACT

In recent years, a large number of indole derivatives have been shown to possess an array of biological properties like anticonvulsant, anti-depressant, antihistamine, antidiabetic, etc[1-3]. 1,2,4-Triazoles are well known compounds and are found to possess varied pharamacological activities. The analgesic, diuretic, antiviral antibacterial, and antifungal properties exhibited by various 3-substituted-5-mercapto-1,2,4-triazoles. Further Indole associated with active heterocycles like imidazole, thiazole, oxazole etc. at 3-position has reported promising potent biological activity[4].

Keeping in view of above, it was thought fit to synthesize Indole derivatives containing 1,2,4, Triazole at 3-position.

Condensation of 3-substituted-4-amino-5-mercapto-1,2,4-triazole and 5/6-subtituted-Indole-3-carbaldehyde in ethanol and catalytic amount of conc. HCl, yield Schiff bases. Interaction of the resultant schiff's bases with suitable active primary/secondary amine in ethanol and formaldehyde gave title compounds.

The newly synthesized compounds were characterized by spectral data. Screening of anti-inflammatory, analgesic and anti microbial activity of newly synthesized compounds is under progress.

PP-383

Plant extracts: A potential source of antifungal compounds

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ABSTRACT

In the present study antifungal activity of L. inermis leaf and E. citriodora leaf against toxigenic strains of Aspergillus flavus and A. parasiticus has been assayed Steyn . Bioassay of various extract was done with respect to seed germination, seedling growth i.e. radical and plumule elongation in peanuts seeds.Antifungal activity of crude alcohol, 50% hydro-alcohol and aqueous extracts as well as partially purified fractions of the crude extracts has been assayed against both test fungi Cowan et al.Acetone was used to dissolve various fractions prior to antifungal screening. Acetone fraction of L. inermis leaf and PE fraction of E. citriodora leaf showed best antifungal activity. These fractions were subjected to separation by column chromatography. Leaf fraction 1 of L. inermis and fraction no. 1-4 of E. citriodora leaf exhibited good antifungal activity against all the test fungi. Bavistin and mancozeb were used as standard synthetic antifungal for the comparison. Minimum fungi-static and minimum fungicidal concentration of all extracts was also determined. Phytotoxicity testing of extracts of leaves proved them non toxic to peanuts and maize grains Shukla et al . Results suggest the potential use of these plant parts (leaves, flower, bark and stem) as an eco friendly antifungal and safer alternative for safe storage of grains.

PP-384

Complex Formation of *Brugia malayi* Calreticulin with Human C1q (BmCRT-HuC1q) Blocks Activation of Human Complement System

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ABSTRACT

Most biological processes in living organism are regulated by an intricate network of protein-protein interaction and many of these pathways are deeply involved in diseases. Therefore, current research in biomedicine is focusing on a detailed knowledge of these interactions at molecular level which are necessary for drug discovery. In classical complement system after the interaction of IgG/IgM with C1q a sequential activation of C1q-bound C1r and C1s serine proteases promote proteolysis of C_4 to produce C4b,that is responsible for complement cascade activation(MAC).Therefore, compounds that interfere with the C1q-$C1r_2C1s_2$ interaction will cause inhibition of classical pathway. Calreticulin of Filarial parasite, *Brugia malayi* (BmCRT) has the ability to block complement system of host by complex formation with C1q first component of host complement system.BmCRT-HuC1q complex prevents cleavage of C4 into C4a and C4b causing inhibition of the entire cascade .The properties of human filarial parasite, Calreticulin have not been studied and hence studied were conducted to characterize the protein and understand its role in host-parasite interaction. The BmCRT was successfully cloned, expressed and purified by Ni-NTA column .The interaction of the purified protein with human C1q was studied under in vitro conditions .Novel Interaction of BmCRT with HuC1q inhibited the C1q dependent lyses of immunoglobulin-sensitizes Red Blood Cells. Ca^{+2} played a significant role in complex formation and its stability. These findings signify that BmCRT may be a key factor contributing to ability of parasite to interfere at the earliest stages of complement activation which may help infectivity of parasites and long live host-parasite relationship.

PP-385

Plastid as drug target in malaria parasites

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ABSTRACT

From decades malaria has remained a major disease, inflicting illness in millions of humans around the world. It is caused by an apicomplexan parasite *Plasmodium.* A number of drugs including Chloroquine, pyrimethamine, sulfadoxine and latest one Artemisinin and its derivatives are being used for treating this disease but past few years have seen a rise in the cases of drug resistance in the parasite. Thus, there arises a need to search novel & effective drug targets. Malaria parasite harbors a plastid like organelle termed apicoplast, having a circular genome which is highly conserved among different parasite species and other apicomplexans. The genome construction is similar to that of chloroplast DNA but is devoid of photosynthetic genes making this organelle non-photosynthetic. The organelle is a site for some crucial, prokaryote specific metabolic pathways. Thus, the enzymes participating in these pathways can be specific drug targets. Mcfadden et al. [1].

Apicoplast, its genome and metabolic pathways have been extensively studied in *Plasmodium falciparum.* We are the first group to characterize and report the sequence of almost 55% plastid genome from *Plasmodium vivax.* The functions of major genes encoded by the genome are still hypothetical. However, till date functions of only one gene from *P.falciparum* plastid genome has been elucidated experimentally i.e. tuf A that encodes for elongation factor EF-TuA. The gene is highly conserved and has binding sites for tRNAs and certain antimicrobial compounds like kirromycin and amythimicin. Saxena et al. [2]. Through immune-fluorescence technique we have characterized *P.vivax* plastid *tuf A* gene which seems to be translationally active within the apicoplast.

PP-386

Synthesis of 2-aryl-1-arylmethyl-1H-benzimidazoles using chlorosulfonic acid at room temperature

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ABSTRACT

Chlorosulfonic acid (ClSO3H) used to be a catalyst for the synthesis of 2-aryl-1-arylmethyl-1H-benzimidazoles which was ef?ciently simple and convenient. This method afforded short reaction time, easy workup, moderate to excellent isolated yields which make this protocol practical and economically attractive.

PP-387

TASK SPECIFIC IONIC LIQUID IN CYCLOADDITION REACTION: A HIGHLY SELECTIVE APPROACH FOR THE CONSTRUCTION OF NOVEL DISPIRO HETEROCYCLES

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ABSTRACT

In recent years, Ionic liquids (ILs) have received recognition as a new generation of solvents having unique physicochemical properties, such as nonvolatility, excellent chemical and thermal stability, nonflammability, and good solvating ability, Their dual organic and ionic nature allows them to establish ion-ion and ion-dipole as well as van der Waals interactions with reacting species, including transition states; hence they sometimes give rise to improved yields and rate enhancements. These unique properties of RTILs have led to their use as molecular tools in synthetic chemistry.

In continuation of our ongoing program in the development of greener and sustainable process for the synthesis of spiroheterocycles and our expertise in cycloaddition reaction, herein, we wish to report for the first time, a highly efficient and green protocol for the synthesis of pharmaceutically important novel dispiropyrrolidines *via* three component reaction of ninhydrin, sarcosine and 1-benzyl/methyl-3,5-bis[(*E*)-arylidene]-piperidin-4-one using task-specific [TMG][Ac] ionic liquid as

the recyclable solvent. The TMG-based ionic liquid could be recovered and used at least four times without considerable reduction in its activity and selectivity. Good functional group tolerance and broad scope of usable substrates are other prominent features of the present methodology with high degree of chemo-, regio- and stereoselectivity. The structure and relative stereochemistry of final products was established by single crystal X-ray structure and spectroscopic techniques.Detailed synthetic methodology and biological activities of these compounds will be presented in the conferences.

PP-388

Moxidectin demonstrates profound macrofilaricidal activity against *Brugia malayi* when used alone or in combination with other filaricides

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ABSTRACT

Moxidectin (MOX) is a macrocyclic lactone progressing towards Phase III clinical trial against *Onchocerca volvulus.* The present study was therefore designed to evaluate the *in vitro* and *in vivo* antifilarial efficacy of MOX in combination with filaricides- Diethylcarbamazine citrate (DEC) and Albendazole(ALB) as also the anti-wolbachial antibiotic- doxycycline (DOXY) against lymphatic filarial parasite, *Brugia malayi* at various concentrations on both the life-stages MOX *in vitro* showed 100% reduction in worm motility at 5 μM concentration within 48 h of exposure. MOX was also effective at concentrations lower than 5 μM when the drug exposure time was extended up to 10 days. The IC50 of all the drugs used in the present study and different drug combinations was found to < 5 μM and therefore all these combinations were followed in *in vivo* primary screening model i.e. intraperitoneally adult *B. malayi* transplanted jird model. MOX administered subcutaneously showed 85.36% reduction in adult worm recovery. The response of other filaricides or antibiotic in combination with MOX showed nothing better than MOX alone. The present findings therefore indicate that *in vitro* exposure of parasite to a combination of moxidectin with albendazole or doxycycline had superior antifilarial activity than when used alone while *in vivo* MOX alone showed best response.

PP-389

Synthesis and bioevaluation of triazole derivatives of 2-cyano pyrrolidine: as anti-diabetic agents

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ABSTRACT

There has been ever-increasing need for rapid reactions that meet the three main criteria of an ideal synthesis: efficiency, versatility, and selectivity. Such reactions would allow medicinal chemistry to keep pace with the multitude of information derived from modern biological screening techniques. The 1, 3-dipolar cycloaddition (''click-reaction'') between azides and alkynes catalyzed by copper (I) salts [1]. The simplicity of this reaction and the ease of purification of the resulting products have opened new opportunities in generating vast arrays of compounds with biological potential. By consideration of utility of click chemistry reaction in medicinal chemistry for development of huge library of biologically active compounds, we decided to synthesize the DPP-4 Inhibitors, a potent antidiabetic compounds which are lacking the stability and selectivity [2]. In view of the importance of 2-cyano pyrrolidine scaffold and structural similarity with vildagliptin, we have designed and synthesised various triazole derivatives of 2-cyano pyrrolidine for the evaluation of DPP-4 agonism studies. Vildagliptin and all the other DPP-4 inhibitors have less stability because of intermolecular cyclization and hence the half lives of these drugs are very less [3]. So we decided to insert bioisostere in the drugs for improving the pharmacokinetic profile. So based on the result of docking studies on the GLIDE software we finalised different molecules with high binding score. Click chemistry is the main reaction that is used for the synthesis of the different triazole analogues [4- 6]. We have checked the *in vitro* antidiabetic activity of these compounds by the DPP-4 enzyme inhibition.

PP-390

"Recent Advances and Current Trends in Chemical and Biological Sciences" The root extract from 101R chemotype of *Withania somnifera* and the pure molecule, Withaferin A protects the host against *Brugia malayi* by immunostimulation

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ABSTRACT

Withania somnifera is an Ayurvedic Indian medicinal plant whose immunomodulatory activities have been widely used as a home remedy for several ailments. We recently reported immunostimulatory properties in the root extracts of chemotypes NMITLI-101, NMITLI-118, NMITLI-128 and pure withanolide, Withaferin A (Kushwaha et al, 2012). These findings prompted us to further investigate the immunoprophylactic efficacies of these agents against infective larval challenge with human lymphatic filarial parasite, *Brugia malayi*. Oral treatment of *Mastomys coucha* with 10 mg/kg of each extract or 0.3 mg/kg of Withaferin A for 7 consecutive days just before infective larval challenge and for subsequent 7 days (14 days total) offered various degrees of protection against *B. malayi*. The chemotype 101R offered best protection (53.57%) amongst the three chemotypes while Withaferin A exhibited marginally superior protection (63.6%) in terms of recovery of adult filarial parasites, microfilaraemia and female worm fecundity (66.2%). The filaria-specific immunological responses induced by Withaferin A and NMITLI-101 were almost similar with mixed Th1/Th2 phenotype, 118R stimulated production of IFN-? (Th1) while 128R treatment led to increased IL-4 level. Taken together, the findings reveal that selection of chemotype is critical to achieve the desired biological activity and 101R chemotype proved to be promising where the activity was located in the single molecule, Withaferin A. Further studies would help to ascertain the benefits of this plant against other pathogens as well.

PP-391

Wolbachia Surface Protein (WSP) Of *Brugia malayi* Endosymbiont Contributes To Host Inflammatory Response By Modulating Th1/Th17/Treg Cells

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ABSTRACT

Endosymbiont bacterium *Wolbachia* present in the major human filarial species has been indicated to contribute to filarial immunobiology and pathogenesis. Wolbachia surface protein (WSP) has been considered to be involved in producing inflammatory pathology in the host. It is widely recognized that the Regulatory T cells (Treg) expressing the transcription factor Foxp3+ controls the components of the immune system. The proportion of Treg cells is reciprocally related to that of pro-inflammatory T cells producing interleukin-17 (TH17). The involvement of WSP in TH17/Treg cell response is still poorly understood and also the exact mechanism of up-regulation IL-17+ expression is not known. In the present study, we PCR amplified the WSP gene, cloned it , over-expressed it as a single band at ~25 kDa. The protein was brought in to soluble form and administered in to BALB/c mice for studying the immune response generated by the recombinant protein of Wolbachia. We further investigated the role of WSP as a regulator of TH17 and Treg differentiation in mice. WSP immunization induced functional TH17 cells along with TH 1 cytokines. On the other hand, it also interfered with the Treg cell development, and this effect increased after challenging the animals with infective larvae (L3) of B. malayi. There was more pronounced expression of TH 17 and down regulation of Treg. The real time monitoring of Foxp 3 and IL-17 further confirmed this phenomenon. This is the first direct evidence of generation of proinflammtory response by WSP via downregulation of Treg population and up-regulation of TH17 cells.

PP-392

Bionematicide: A safer way to control root knot nematode *Meloidogyne incognita*

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ABSTRACT

Present study deals with assay of nematicidal activity *Adhatoda vasica* leaf and inflorescence extract against root knot nematode *Meloidogyne incognita* with an aim for isolating and identifying a novel nematicide as well as paving the way for development of an eco-friendly herbal bio-control formulation. Zia et al [1]. *In vitro* nematicidal assay of crude 100% alcohol, aqueous and 50% hydroalcohol extract and partially purified extracts of *Adhatoda vasica* was assayed by egg hatching and larval mortality methods.Singh et al.[2]. *In vivo* effect of *Adhatoda. vasica* was studied by performing pot experiments using powdered plant material and/or extract as soil amendment and bare root dipping treatment with tomato and brinjal as host plants. Mojumder[3]. Histopathology of roots of healthy, infected host plant and plants treated with plant material/extract was also done. Change in anatomy of root, formation of giant cells, abnormalities in xylem and phloem cells etc. were observed microscopically and documented. The effect of plant extract/ dried powder on host plant growth, shoot length, root length, fresh and dry weight of shoot and root, number of galls/plant and final nematode population in soil were measured. Reduction in root galls and nematode population in tomato and brinjal indicates that the *A. vasica* leaf powder and alcohol extract inhibit egg hatching and larval development of *M. incognita* and increase plant growth parameters. Highest reduction in root-knot development was observed with combined application of soil amendment with leaf powder and bare root dipping with alcohol extract followed by soil amendment and bare root dipping individually.

PP-393

Synthesis, Antiproliferative, and c-Src kinase Inhibitory Activities of Chromen-2-one Derivatives

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ABSTRACT

Although a lot of progress has been made in developing anticancer agents, cancer still remains an enormous threat to people's health in the 21st century. Thus, there is need to design anticancer agents with higher therapeutic index. The inclusion of the distinct pharmacophores of two different biologically active compounds in the same structure, also known as 'medicinal chemistry hybridization', has been attempted in a successful manner to enhance the therapeutic index[1-2]. Earlier we had explored the biological activity of individual chalcone and coumarin moiety and found promising results[3-6], so in this perspective and to explore the chemical diversity space around chromen-2-one and chalcone scaffolds, our research group has blended the two pharmacophores in one unit by synthesizing novel cinnamoyl- and pyranochromen-2-one derivatives. The antiproliferative activity of these compounds was evaluated towards colon adenocarcinoma (HT-29), breast carcinoma (MCF-7), human ovarian adenocarcinoma (SK-OV-3) cell lines, and Src kinase inhibition. A few of these compounds were found to be consistently active against all the three cancer cell lines and also exhibited the highest Src kinase inhibition. The preliminary interesting results would be presented as a poster.

PP-394

Glucose: A Better Alternative Reductant for Copper-Catalyzed Azide Alkyne Cycloaddition (CuAAC) reactions

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ABSTRACT

An exergonic fusion to form triazole ring *via* azide alkyne cycloaddition (AAC) reactions has enjoyed its legacy in drug discovery, bioconjugation and materials science[1] since the first synthesis of 1, 2, 3-triazole (*v*-triazole) from phenyl azide and acetylene dicarboxylic ester was reported by A. Michael[2] in 1893, followed by F. Holder[3] and K. Raschig.[4] Tolerance of various azides and alkynes for the formation of *v*-triazoles was excellent, however these cycloaddition reactions showed very

low regioselectivity and yielded a mixture of 1, 4- and 1, 5- regioisomers.[5] The improvement of the poor regioselectivity of dipolar cycloaddition involving azides and alkynes was an attractive and challenging target till 2002, when Fokin & Sharpless proposed a historic Cu (I) catalyzed protocol for regioselective cycloaddition reaction.[6] In 2002 they described a mild and convenient Cu (I) catalyzed protocol for the synthesis of.1, 4 – regioselective isomer. Subsequently, they also observed that *in situ* reduction of Cu (II) salt by sodium ascorbate to be a better choice as compared to direct use of Cu (I) source.[1g]

Very recently, we have established D-glucose as reductant for the Copper Azide Alkyne Cycloaddition (CuAAC) reactions (Scheme given below). Efficacy of this inexpensive reductant has been established by using various phenyl acetylenes and aryl azides. All reactions proceeded smoothly and 1, 2, 3 – triazolyl derivatives were obtained in moderate to excellent yields (61 – 95 %). Deatils of this protocol would be presented in the at the meeting.

PP-395

Microwave assisted synthesis of piperidine/piperazine based chalcones and their antiparasitic evaluation against *Giardia intestinalis*

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ABSTRACT

Giardiasis is a worldwide waterborne intestinal parasitic disease, caused by the amitochondriate protist *Giardia intestinalis*[1]. This microaerobic, flagellated unicellular eukaryote, first discovered by the Dutch microscopist Antony van Leeuwenhoek in 1681, has a relatively simple life cycle. It spreads in the environment as a stable, highly infectious cyst; once ingested by the host, it reaches the stomach lumen and develops into its vegetative form, the trophozoite, that attaches to the intestinal epithelium and starts proliferating in the proximal small intestine, eventually causing the disease. Here this microaerobic parasite must survive exposure to O_2, nitric oxide (NO) and related reactive species, most likely through the intervention of a battery of detoxifying enzymes [2]. Following encystation, the parasite is finally expelled back to the environment, ready to infect other hosts.

Library of novel chalcones of total of forty-eight compounds were synthesized by microwave assisted Claisen-Schmidt condensation,[3] purified and characterized by high resolution mass spectrometry, ^{1}H and ^{13}C nuclear magnetic resonance and infrared spectroscopy. The Anti Giardial activity of all the synthesised compounds has been done. The details of the activity will be illustrated later.

PP-396

CHIRAL PHTHALIMIDES WITH GREATER SECOND HARMONIC GENERATION RESPONSE

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ABSTRACT

Design and synthesis of organic molecules possessing significant second harmonic generation response is of great interest owing to their versatile applications in the field of existing and future technologies. Organic materials are always preferred in material science due to their easy tailoring and high solubility over pure inorganic materials. A series of small chiral phthalimides have been designed and synthesized with the aim to explore their structural features and their nonlinear optical properties. The composition of newly prepared molecules was confirmed by analytical and spectroscopic techniques and also by single crystal X-ray diffraction technique. The molecules were evaluated for their first molecular hyperpolarizabilities (?). The polycrystalline samples were subjected to Kurtz-Perry powder test for measuring second-harmonic generation response. The interesting and enthusing results are observed and will be presented.

PP-397

Identification of Cosavirus by Metagenomics and Prevalence in Stool samples of Children with Acute Flaccid Paralysis, India.

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ABSTRACT

Although wild poliovirus has been eradicated from India, increasing acute flaccid paralysis (AFP) cases without identified etiology are reported in polio endemic region which is of serious concern. To characterize the viruses circulating in this population we used sequence-independent single primer amplification (SISPA) of partially purified viral nucleic acids from stool samples of nonpolio AFP children tested negative for virus isolation according to WHO standard methodology. SISPA was performed on fecal samples from children <15 years age diagnosed with AFP. Limited Sanger sequencing was conducted for randomly amplified PCR fragments of size between 100-450 bp. We identified RNA fragments related to a recently discovered virus, human cosaviruses (HCoSVs) (family *Picornaviridae*) (Kapoor et al. [1]). The information about the detection and prevalence of this virus in India is currently unknown. Therefore, we investigated the prevalence of this virus in nonpolio AFP cases. A total of 15 stool samples from 47 nonpolio AFP children analyzed were RT-PCR positive for cosavirus with primers directed to 5'UTR and RdRp region. Phylogenetic analysis concordant in both regions indicated the presence of cosavirus species A in majority of the positive samples (13/15), showing dominance of HCoSV-A species circulation in India while sequences of 2 positive samples did not cluster with known cosavirus species. This study reports the first investigation of HCoSV infection in nonpolio AFP children in polio endemic region with prevalence of 32%. Further studies are needed to examine the roles of these HCoSVs and their different viral protein 1 (VP1) genotypes in nonpolio AFP and other human diseases.

PP-398

Evaluation of antidiabetic activity in ethanolic extract of *Allium cepa* bulbs

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ABSTRACT

Allium cepa (*A. cepa*), family: *Liliaceae* is commonly known as garden onion or bulb onion, an edible plant in Ayurvedic and Indigenous Medicinal System. The crude powder of the bulbs of *A. cepa* was extracted with 95% ethanol by percolation method. The ethanolic extract was evaluated for antidiabetic activity on skeletal muscle cell line (L-6) and on validated animal models of diabetes mellitus. The ethanolic extract of bulbs of *A. cepa* showed 21.4 % ($p<0.01$) improvement of oral glucose tolerance on normal rats and 22.7% ($p<0.01$) and 19.6% ($p<0.01$) decline on blood glucose levels at 05h and 24h, respectively on streptozotocin-induced diabetic rats at 250 mg/kg body weight dose. The ethanolic extracts also increases glucose utilization by L-6 muscle cells in dose dependent manner. To exp lore the antidiabetic mechanism(s) of *A. cepa* extract on expression profile of selected genes in L6 myotubes, cells were treated with 10µg/ml of the extract for 16 hours. Total RNA was isolated and gene expression was analysed by RT-PCR which showed down-regulated expression of PPAR ?, PDK4, and PDK2. The expression of PGC-1a, PGC-1ß, Cox 7 and PFKm was found to be up-regulated. The differential regulation of metabolic genes and transcription factors involved in carbohydrate and fat utilization (Jeoung et al. 2010 [1]) will give greater insight into the molecular basis of development of metabolic disorders like diabetes mellitus. The results of the present study show that ethanolic extract of *A. cepa* bulbs has promising antidiabetic potential for further investigation.

PP-399

Synthetic and biocidal studies on oxovanadium complexes of substituted 2-pyrazolines having thienyl moiety.

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ABSTRACT

The oxovanadium (IV) complexes of 1-acetyl-5-aryl-3-(substituted thienyl)-2-pyrazolines have been synthesized. The structures of the isolated complexes have been elucidated on the basis of elemental analysis, molecular weight determination, molar conductance, magnetic moment and spectral (ESR, IR and UV) data. The ligand behaved as bidentate coordinating through carbonyl oxygen and azomethine nitrogen. The ligands exhibited significant in-vitro microbiocidal activity against phytopathogenic fungi viz., Alternaria altemata, Collectotrichum Capsicum, Fusarium oxysporum, Rhizoctonia solani & bacteria viz. Bacillus subtilis and E.coli which was significantly enhanced on metalation.

PP-400

Exploring the Possible Mechanism of Action for Anti-Inflammatory Potentiality of Extracts of *Bridelia Retusa Spreng* (Bark)

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ABSTRACT

Background & Objective: *Bridelia retusa spreng* (*B.retusa*) belonging to the family Euphorbiaceae is a tree or a shrub approx 17-18 m in height fortified with sharp and strong spines. High levels of in?ammatory cytokines like Interleukin-6 (IL-6) and Tumor necrosis factor alpha (TNF-a) are proposed contributors to the pathophysiological mechanisms associated with various in?ammatory disorders. The modulation of their production may be an effective therapy for the treatment of inflammatory diseases. The present study sought to explore the possible mechanism of action for anti-inflammatory potential of the extracts of *B.retusa* bark. Methods: Extracts prepared from solvents of different dielectric constant were subsequently screened for their anti-inflammatory potential in various anti-inflammatory models namely Carrageenan-induced rat paw edema method (Acute), Formalin induced rat paw edema (For accessing the arthritic potential) and Cotton pellet induced granuloma (Chronic). The molecular levels of Tumor necrosis factor- alpha (TNF-a) and Interlecukins-6 (IL-6) were determined quantitatively using the Enzyme Linked Immunosorbent assay (ELISA) kit. Results and Conclusion: Chloroform and the methanolic extracts possessed significant anti-inflammatory activity in Carrageenan, formalin and cotton pellet induced granuloma. In the methodology adopted for estimation of IL-6 the chloroform at 70 mg/kg produced significant inhibition of 29.7±0.02 ($P<0.05$) and at 140mg/kg produced inhibition of 44.2±0.21 ($P<0.01$). In TNF-a estimation the methanolic extract at 70mg/kg and 140 mg/kg produced inhibition of 18.2±1.27 ($P<0.05$) and 22.3±1.81 ($P<0.01$). Chloroform extract inhibited IL-6 more efficiently as compared to TNF-a and methanolic extract produced better results in TNF-a inhibition as compared to the chloroform extract. It can be inferred that the possible mechanism of action of the chloroform extract is towards inhibition of IL-6 and realizing the dominant activity of methanolic extract towards inhibition of TNF-the mechanism of action predicted for methanolic extract can be the suppression of TNF- a. The result of the present investigation affirms the presence of pure bioactive metabolite from a natural origin in the chloroform and the methanolic extract of the bark of *B.retusa*. The said extracts could serve as a valuable source for the isolation of a chemotherapeutic agent with a potent anti-inflammatory activity. This investigation provides scientific rationale for the use of bark of *B. retusa* as a remedy for gastrointestinal, skin and fungal infections in folkloric medicine.

PP-401

Synthesis of pyrimidine analogues of triazole linked chalcone

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ABSTRACT

Chalcones are products of condensation of aromatic aldehydes with acetophenones in the presence of alkali. Chalcones and their derivatives constitute an important group of natural products and are an attractive molecular scaffold for the search of new biologically active molecules.[1] A number of chalcones having hydroxy, alkoxy groups in different positions have been reported to possess antimicrobial, anticancer, antitubercular , ,antiviral etc.[2]

In view of pharmacological properties, we herein report the synthesis of triazole linked chalcone derivatives with an aim to develop new antibacterial agents with novel structure. The antimicrobial activity of these compounds were evaluated *in vitro* by disc diffusion method against gram positive and gram negative bacterial strains compared to gentamycin.[3]

PP-402

PHARMACOPHORE MODELING, DOCKING AND SYNTHESIS OF SMALL ORGANIC MOLECULES AS ANAPLASTIC LYMPHOMA KINASE INHIBITORS FOR THE TREATMENT OF NSCLC

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ABSTRACT

Lung cancer is one of the most widespread diseases and cause for death in India. The main cause of lung cancer is tobacco but now it has been found that air pollution also causes lung cancer. Sanghita et al. [1] It is divided into two classes - non small cell lung cancer(NSCLC) and small cell lung cancer(SCLC). Jair et al. [2] Anaplastic lymphoma kinase(ALK) is mainly involved in NSCLC. ALK is a receptor tyrosine kinase which belongs to the insulin receptor superfamily and has emerged as a prominent target for the NSCLC therapy. ALK is normally expressed in CNS and was originally identified as a component of several fusion protein nucleophosmin (NPN)-ALK. Craig et al. [3] This fusion kinase plays oncogenic role in anaplastic large cell lymphomas. Promising compounds from literature were selected for the generation of a pharmacophore using GASP module of SYBYL X 1.2. Rabindranath et al. [4] A four component pharmacophore model consisting of a hydrogen bond donor, a hydrogen bond acceptor and two hydrophobic groups was generated and validated using ROC curve methodology. On the basis of this pharmacophoric model virtual screening of selected compounds from NCI database was carried out. 10 best Qfit score compounds were taken as best compounds for docking study which showed good interaction with the enzyme. Five new compounds were designed on the basis of the pharmacophore model and docking was performed. In silico ADME properties of the five compounds were calculated by OSIRIS online tool. Synthesis of two of the best five compounds was carried out and their structure elucidated using spectral studies.

PP-403

2-(1-Benzotriazolyl)pyridine: A Robust Bidentate Ligand for the Palladium-Catalyzed C–C, (Suzuki, Heck, Fujiwara-Moritani, Sonogashira), C–N and C–S Coupling Reactions

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ABSTRACT

Our recent success on the coupling reactions using benzotriazole as a ligand,[1] motivated us for the designing of more efficient and practical ligand for the palladium-catalyzed coupling reactions. A new type of bidentate ligand, 1-(pyridine-2-yl)-1*H*-benzo[*d*][1,2,3]triazole have been designed and employed for the palladium-catalyzed C–C (Suzuki, Heck, Fujiwara-Moritani, and Sonogashira), C–N and C–S coupling reactions. The ligand found to be inexpensive, thermally stable, easy to synthesize from easily accessible starting materials in multigram scale, simplicity in use, and robustness in application, making this ligand effective for different coupling reactions. Suitably, the donor ability of *N=N* of benzotriazole ring and lone pair of *N* of the pyridine ring enhance the bidentate ability of the ligand.

PP-404

Efficient solvent- free synthetic methods using zinc oxide as a heterogeneous and reusable catalyst at room temperature

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ABSTRACT

Chemical processes on metal oxide surfaces have been of great interest for a long time, mostly due to their relevance in the field of heterogonous catalysis. It is widely believed that the high reactivity of oxide powders results from the presence active sites on the surface Henrich et al [1]. As the surface have properties that are not duplicated in the solution or gas phase,

entirely new chemistry may occur. The surface reaction may be more desirable than a solution counterpart, because the reaction is more convenient to run or a high yield of product is attained Toda et al [2]. Experiments using the solid-phase catalyst generally have the features: (i) it is easy to isolate the products and to separate the catalyst; (ii) comparing the reaction conditions with those of related homogeneous reactions, they are so mild that a high yield of specific products, and (iii) selectivity and activity of the catalysts Pagni et al. [3]. Zinc oxide (ZnO) is an inexpensive and commercially available inorganic solid has been used as a catalyst in number of chemical transformations. Herein, we report a new, simple, and regioselective synthesis of chalcones More et al. [4] and thiol esters Bandgar et al. [5] using ZnO as a catalyst under solvent-free conditions at room temperature.

The catalyst was recovered by simple filtration. In order to study, catalytic activity of recovered catalyst (ZnO), it was reused at least three times in the reaction. Furthermore, the selectivity of the catalyst (ZnO) was examined.

PP-405

Study of Antioxidant, Aldose Reductase Inhibiotion and Anti-cataract activity of *Tinospora cordifolia*: Prospects for alleviating diabetic complications

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ABSTRACT

Phytotherapy has played an important role in the management of diabetes and related complications. Diabetes mellitus represents the final consequence of a chronic and progressive syndrome. The cost of diabetes treatment and associated complications has great implications and therefore preventive measures are important.

In the preent study, the antioxidant, anti-cataract and anti-glycation properties of stem extract of *Tinospora cordifolia* were evaluated using *in vitro* standard procedures. The antioxidant activity was determined by DPPH (1,1-Diphenyl-2-picrylhydrazyl) radical scavenging assay (IC_{50} 3981µg/ml and 602.6µg/ml for aqueous and alcoholic extract respectively) and FRAP (Ferric reducing antioxidant power assay). The extract showed significant decrease in protein oxidation when the lysozyme and GLP (Goat Lens Protein- 6mg/ml) were incubated with 200mM and 100mM glucose along with 2.75mg/ml plant extract as compared to those without plant inhibitors. The goat lens opacity model showed that with increase in concentration of plant extract (250µg/ml and 1000µg/ml), the opacity of the lens goes on decreasing.

Thus, the present study suggests that *Tinospora cordifolia* stem extract may be used as an anti-cataract and anti-glycation agent. Further its anti-diabetic potential must be evaluated.

PP-406

Synthesis of some novel ß-diketones and ß-ketoesters of 4-methyl sulphonyl benzoyl methylene bromide

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ABSTRACT

The importance of ß-diketones/ß-ketoesters in synthetic organic chemistry is difficult to overstate. ß-diketones/ß-ketoesters are stable, usually nontoxic and therefore convenient for storage and use. It is mainly due to their high reactivity that predetermines them for synthesis of various types of compounds particularly heterocycles such as diazepines[1], benzodiazepines[2], benzothiazepines[3], benzothiazines[4], pyrazole[5], imidazole and benzimidazol[6].

Various novel ß-diketones and ß-ketoesters (4a-e) have been prepared by the condensation of 4-methyl sulphonyl benzoyl methylene bromide (2) with ß-diketones and ß-ketoesters (3a-e) in the presence of sodium methoxide in dry toluene. Reaction mixture was heated for about twenty two hours at 80 °C with proper stirring. The progress of the reaction was monitored through TLC using benzene: ethanol: ammonia (7:2:1), upper layer as mobile phase. The structure of newly synthesized compounds have been elucidated by elemental analysis, IR, ^{1}H NMR and ^{13}C NMR studies.

PP-407
In-Vitro and In-Vivo Characterization of Engineered Docetaxel Nanocrystals based on Pluronic F-127

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ABSTRACT
In an attempt to develop a more safe and effective docetaxel parenteral formulation for the treatment of breast cancer, docetaxel nanocrystals (NCs) were prepared using pluronic F-127 as a base stabilizer. Docetaxel NCs were prepared by three phase nanoparticle engineering technology and were characterised for particle size, polydispersity and zeta potential. The formation of NCs was confirmed by X-ray diffraction studies. The aggregation of docetaxel with pluronic F-127 was affirmed by UV-visible spectroscopy based aggregation study and differential scanning calorimetry. The developed NCs were also evaluated for haemolytic activity using blood and in-vitro cytotoxicity in MCF-7 cell line. The particle sizes of the developed NCs were in ranged between 193.3±10.4 to 932.1±21.5nm with polydispersity index range from 0.281±0.012 to 0.938±0.065 which ensures the suitability of the developed formulation for parenteral administration. The zeta potential of the NCs was found in the range from -10.6±2.21 mV to -20.7±1.54 mV indicating the stability of the NCs. Free drug, NCs and marketed formulation (Taxotere) showed 12.585± 0.449%, 3.112±0.693% and 17.15818± 0.986% haemolysis respectively after 4h of incubation. The NCs were found to commit improved efficacy compared to free drug and marketed formulation in MCF7 cell line. Moreover, in-vivo acute toxicity studies demonstrated that the developed NCs and marketed formulation are safer than the free drug at therapeutic dose of docetaxel. These results together elicit that NCs may have high potential for alternative more safe and effective delivery system for parenteral administration of docetaxel in the treatment of breast cancer.

PP-408
Base-Mediated Selective Intermolecular Addition of Heterocyclic Amines onto Alkynes and Alkynones

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ABSTRACT
Hydroamination of alkenes, alkynes, and related unsaturated substrates represents an attractive strategy for the construction of nitrogen-containing compounds that almost prevents the formation of by-products in the creation of a C-N linkage [1]. In continuation of our recently developed method for tandem synthesis of indolo- and pyrrolo[2,1-*a*]isoquinolines [2], we have described a versatile and efficient regio- and stereoselective synthetic method to produce a broad range of functionalized vinyl- and styryl enamines [3] which are useful as synthetic intermediates to synthesize biologically active compounds. This metal and ligand free methodology utilizes a simple and economical base KOH for the addition of N-heterocycles not only onto terminal and internal alkynes but also for 1,3- and 1,4-dialkynes. Addition of heterocyclic nucleophile onto alkynones has also been reported under mild conditions.
Current work also supports and confirms the mechanistic pathway for the copper catalyzed synthesis of indolo- and pyrrolo[2,1-*a*]isoquinolines via formation of *Z*-stereoisomer by hydroamination of *ortho*-haloarylalkyne followed by oxidative addition in the presence of metal and ligand [3b].

PP-409
Synthesis of Chitosan Hydroximate Resin for the Selective Adsorption of Metal Ions

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ABSTRACT
The naturally occurring biopolymer, chitosan is chemically modified with iminodiacetic acid dihydroximate (IMDAH-CH) to improve its selectivity and capacity for metal ions. The resin was characterized by means of IR spectra, nitrogen content and pH titrations. The resin characteristics viz., bulk density, specific bulk volume, moisture content, degree of substitution and ion exchange capacity were also studied. The distribution coefficient (Kd) values of different meta ions, namely Co(II), Ni(II), Cu(II), Zn(II), Ca(II), U(VI) and W(VI) on the resin are given as a function of pH. The Kd values of IMDAH-CH resin are compared with that of Iminodiacetic acid dihydroximate in guar (IDAAH-G) resin. The IMDAH-CH resin is found to be more efficient than IDAAH-G resin.

PP-410

Selective biocatalytic acylation studies on 5'-*O*-(4,4'-dimethoxytrityl)-2',3'-secouridine :an efficient synthesis of UNA monomer

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ABSTRACT

Unlocked nucleic acid (UNA) has an incomplete ribose ring open between the 2'- and 3'-carbon atoms and is an acyclic analog of RNA (Fig. 1). Thymine UNA was first introduced in 1995 and it has been shown that the structural flexibility of UNA monomers destabilizes the duplexes. The use of siRNA to knock down gene function has truly revolutionized mammalian cell culture studies and holds great promise in therapeutics. Modification of siRNA with UNA nucleotides has shown highly potent gene silencing activity accompanied by low cell toxicity.

Synthesis of monomeric building blocks of UNA, requires selective manipulation of one of the two primary hydroxyl groups at the 2' -and3'-OH positions in the corresponding 5 '-*O*-DMT-seconucleosides. The chemical methods available for the preparation of 2'-*O*-acylated 5 '-*O*-DMT-seconucleoside requires the use of unfriendly chemicals or low temperature and often leads to the formation of a mixture of acylated products, which reduce the yields of the desired compound.

Herein, we report a very high yielding, selective and environment friendly enzymatic methodology for the synthesis of 2'-*O*-acyl-5'-*O*-DMT-2',3'-secouridine from its corresponding dihydroxy acyclic nucleoside and further 2'-O-benzoyl-5'-O-DMT-2',3'-secouridine is converted to phosphoramidite building block of UNA-U.

PP-411

SYNTHESIS, ANTIMICROBIAL AND MOLECULAR DOCKING STUDIES OF CHALCONE DERIVATIVES BEARING BENZIMIDAZOLE MOIETY

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ABSTRACT

Chalcone derivatives have been found to be biologically privileged entities. A series of chalcone derivatives bearing benzimidazole moiety were synthesized and analyzed by various spectral analyses like IR, ^{1}H NMR and MASS. The synthesized compounds were also screened for their antimicrobial activities against broad panel of microorganisms. Molecular docking studies for anti-tubercular activity of chalcone derivatives were carried out against protein receptor enoyl-acyl carrier protein (acp) reductase using GOLD 3.2 program

PP-412

Ameliorative potential of ferulic acid in vincristine induced painful neuropathy in rats

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ABSTRACT

The present study was designed to investigate the effect of ferulic acid (FA), in vincristine induced neuropathic pain in rats. Vincristine (50 mg/kg, i.p. for 10 consecutive days) was administered to induce painful neuropathy in rats. Various pain sensitive tests i.e., pinprick, cold immersion, hot plate and hot immersion were performed on the different days, i.e.,0,1,3,6,9,12,15,18,21 to assess the degree of mechanical and cold hyperalgesia; heat hyperalgesia and allodynia, respectively. The electrophysiological & morphometric evaluation were also performed. The tissue thio-barbituric acid reactive species, reduced glutathione, MPO, TNF a, IL-6, IL-10 and total calcium were measured as the markers of inflammation and oxidative stress. FA (50 and 100 mg/kg *I.P*) and gabapentin (100mg/kg p.o.), was administered for 21 days. Administration of FA attenuated vincristine induced mechanical, heat and cold hyperalgesia and heat and cold allodynia along with electrophysiological & morphometric changes. FA also attenuated vincristine induced increase in oxidative stress (TBARS, GSH & total calcium levels) and Inflammation (MPO, TNF a, IL-6 & IL-10). It may be concluded that FA has ameliorative potential in attenuating the painful state associated with vincristine induced painful neuropathy, which may further be attributed to anti-inflammatory actions with subsequent decrease in oxidative stress.

PP-413

Expression of leukocyte adhesion molecules and phagocytosis in response to Nisin and Vitamin E plus Selenium treatment during acute bovine mastitis

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ABSTRACT

Phagocytic activity (PA) of milk polymorphonuclear cells (PMNs), concentration of interleukin 8 (IL 8) and expression of L selectin and CD 18 on peripheral leukocyte were studied in response to Nisin and Vitamin E plus Selenium treatment in cows inflicted with acute mastitis. The PA activity of the milk PMNs increased and concentration of IL 8 decreased in post treated cows (P<0.05). The expression of L selectin on peripheral PMNs was lower and CD 18 was higher in mastitic cows compared to healthy cows both before and after treatment (P<0.05).Whilst, the mean fluorescent intensity (MFI) of L selectin enhanced significantly in treated cows on day 7 (P<0.05), but CD 18 remained unchanged .The concentration of Selenium and Vitamin E was lower in mastitic cows. Serum Selenium concentration increased significantly in treated cows as compared to pretreatment values (P<0.05).

The results indicate that Nisin and Vitamin E plus Selenium therapy increases the PA and enhances the expression of L selectin and does not interfere with the expression of CD 18, both the parameters are related to enhancement of the mammary defense. Non antibiotic treatment along with Selenium and Vitamin E was effective in reduction of SCC and IL 8 from the inflamed udder compared to standard antibiotic treatment. Hence combination therapy of Nisin and Selenium plus Vitamin E may be recommended for the treatment of mastitis in such farming system where the antibiotics are not allowed. Furthermore development of such combination therapy is important in reducing the antibiotic residue from human food chain.

PP-413

A Journey of Tissue Cultured Plants from Laboratory to Field andClonal Fidelity Analysis

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ABSTRACT

An efficient and rapid regeneration protocols of some medicinal plants viz., *Withaniasomnifera*, *Vitexnegundo*, *Phyllanthusamarus*, *T. indica* have been developed through different explants viz., nodal segments, intermodal segments, shoot tip etc. Proliferation of these differentiated tissues of diverse medicinal plantsmentioned was achieved on Murashige and Skoog (MS) medium supplemented with different concentrations of cytokinin and auxins. Multiple shoots of these plants were achieved on MS medium fortified with BAP, Kn and TDZ separately or in combinations. Elongation of these shoots was obtained after regular sub culturing on the same medium and growth hormones like Gibberellic acid. These shoots were detached from the shootclump and subcultured on rooting medium consisted with reduced strength of MS salts along with different concentrations and combinations of auxins (Indole 3- butyric acid, Naphthalene Acetic Acid). The *in vitro* recreated shoots were rooted best on half strength MS salts medium with Indole 3- butyric acid (0.5 mg/l to 1.5 mg/l). The complete plantlets have been transferred to small thermocol cups containing different potting mixture such as soil, vermi-compost, soil rite along with autoclaved garden soil (1:3) and coco-peat for hardening. Coco-peat gave maximum percentage of survival rate of the plantlets in the nature (90%). The hardened plants were used to validate the clonal fidelity through Inter simple sequence repeat (ISSR) markers in case of *Tylophoraindica*. The dendrogram based on the unweighted pair group method with arithmetic averaging (UPGMA) depicted about 93 % homology between the mother plant and micropropagated plants.

PP-414

$FeCl_3$-Mediated Regio- and Stereoselective Arylation of a-Hydroxyphosphonates with Arenes: Synthesis of Important Phosphonates

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ABSTRACT

The research on organophosphonates, in particular vinylphosphonates, has captured considerable attention, because the compounds exhibit significant biological properties [1] and immense applications in the field of material sciences [2]. In particular, the *?* –aryl substituted vinylphosphonates and dialkyl (diarylmethyl)phosphonates are fairly well employed for the synthesis of natural product turmerone (an aromatic bisabolene sesquiterpene) [3] and as very essential precursors to introduce the diarylethene moiety [2] *via* Horner-Wadsworth-Emmons reactions respectively. Consequently, synthesis of these phosphonates using an inexpensive and easy approach is highly desirable. Although several expensive transition metals (like Pd, Ru, Cu etc) mediated synthesis of organophosphonates attached with different functionalities are known in the literature, the use of iron is not much explored. In this presentation, we report a simple, efficient and economical $FeCl_3$ mediated regio- and stereoselective Friedel-Craft-type arylation of easily accessible a-hydroxy phosphonates with unactivated arenes, where unstable allylphosphonate cations get stabilized by extended conjugation. It provides a straightforward approach to highly demanding stereoselective *?*-aryl substituted vinylphosphonates and dialkyl (diarylmethyl)phosphonates. These reactions proceed under mild conditions, and can operate in the absence of solvent without the generation of copious waste. All the products and their stereochemistries are confirmed by spectroscopic methods (multinuclear NMR). The single crystal X-ray diffraction analysis was also performed for one analogues compound to confirm the stereochemistry.

PP-415

In-vitro, in- vivo anti –dermatophytic activity of Cinnamomum porrectum Roxb.

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ABSTRACT

The present study was conducted to evaluate and establish the claim of antidermatophytic activities of *Cinnamomum porrectum Roxb*. Based on ethno medicinal knowledge and local use of some plants against some common skin diseases, an attempt has been made to assess the anti-dermatophytic property of this plant against ***Trichophyton rubrum, Trichophyton mentagrophytes, Trichophyton tonsurans, Microsporum gypseum*** by inhibition zone agar cup diffusion method (1). MIC and MFC and in- vivo experiments are done according to standard procedure (2, 3). In- vitro and in- vivo results are very encouraging. MIC values ranging between (312 mg – 625 mg) are close to standard drugs. Further work is in progress on the isolation and elucidation of structure(s) of marker compoumd(s) from the plant.

PP-416

Encapsulation of Clotrimazole into Poly-e-caprolactone Nano-particles and its physicochemical characterization

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ABSTRACT

We report encapsulation of Clotrimazole into poly caprolactone nano-particles and its physicochemical characterization. The composite nano-particles (NPs) were prepared by encapsulating Clotrimazole in to Poly–e-caprolactone (PCL), which is a semi-crystalline biodegradable and biocompatible polymer (1). Nano-particles containing Clotrimazole as drug of choice were prepared by solvent displacement method avoiding the use of toxic chlorinated organic solvents. Scanning Electron Microscopic (SEM) analysis showed that the particles prepared in presence of methanol were spherical with solid dense

structure. The average particle diameter was calculated to be 210 ± 10 nm. The polymer encapsulated Clotrimazole was soluble in aqueous solution and showed distinct photo-physical properties. Fourier Transform–Infrared (FTIR) analysis revealed the absorption peaks of the Clotrimazole, which were not observed in the Clotrimazole loaded PCL NPs. This explains that no Clotrimazole had interacted onto the surface of the NPs, but was completely encapsulated in the PCL nano-spheres. XRD analysis revealed the characteristic peaks of Clotrimazole isolated from loaded Nps appeared at a diffraction angle of 2? angle, which indicates that Clotrimazole is in a highly crystalline form. The encapsulation efficiency (%) of Clotrimazole in PCL nano-particles was dependent on drug to polymer ratio. The *in-vitro* drug release profile along with release kinetics and mechanism from the composite NPs were studied under simulated physiological conditions for different incubation periods (2). The drug loaded nano-particles exhibited sustained release properties followed by a slight initial burst release due to drug adsorbed on the nano-particle surface (3).

PP-417

Design and synthesis of novel phenanthridine derivatives as anticancer agents

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ABSTRACT

Cancer is unregulated cell growth forming malignant tumors, and invades nearby parts of the body. In 2007, cancer caused about 13% of human deaths worldwide (7.9 million) according to global cancer statistics. Benzo[*c*] Phenanthridine is naturally occurring alkaloid, which has anticancer activity through PARP-1 inhibition Makhey *et al.,* [1]. Also certain quinoline derivatives which have piperazine at second position exhibit antiproliferative activity Chih-Hua *et al.,* [2]. Many of the research groups predicted and reported that amide group can be replaced with a triazole ring which mimic and behave in the same fashion. The triazole ring exhibit anticancer activity and serves two purposes: (a) it facilitates stronger cap group interactions with the amino acid side chains at the entrance of the HDAC active site; (b) it serves as an isostere to the pharmacokinetically and toxicologically disadvantageous groups such as amide and ketone Chen *et al.,* [3]. Based on this background study, we strategically designed the new chemical entities. We coupled phenanthridinyl piperazines with various methylene triazoles and wanted to explore the synergistic effect of these heterocycles towards anticancer activity. A series of 6-{4-[(1-substituted-1*H*-1,2,3-triazol-4-yl)methyl]piperazin-1-yl} phenanthridine derivatives were synthesized in an effort to prepare novel anticancer agents. Among the synthesized compounds PT-3 and PT-7 were found to be more active compared to the standard drug etoposide. The compounds were synthesized either by microwave irradiation or conventional methods and were characterized by spectral techniques (IR, ^{1}H-NMR, ^{13}C-NMR and LCMS).

PP-418

Biocatalytic Deacylation studies on 3-azido-3-deoxy-4-*C*-acetoxymethyl-1,2-*O*-isopropylidene-a-D-erythro-ribofuranose: Synthesis of *ribo*-LNA Monomers

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ABSTRACT

The use of enzymes in organic synthesis has been widely accepted and lipases are the most frequently used class of biocatalysts in this area. The selectivity of Novozyme®-435 has been demonstrated and employed in the manipulation of a diastereotopic furanose diacetoxy compound as the key step in the synthesis of a bicyclo 3-azido-3-deoxy furanose derivative, which is an important intermediate for the synthesis of modified oligonucleotides ß-D-ribo-LNA.

The synthesis of nucleoside analogues is of great interest because of their application as a key intermediate for the antisense and / or antigene molecule to regulate targeted gene expression, as well as their direct use for an anti-tumor or an antiviral compound.

3'-Amino-3'-deoxynucleoside is an essential component of oligonucleotide N3'? P5' phosphoramidate that are well known to have high binding affinity with ssRNA, ssDNA and dsDNA.We have efficient by achieved the enzymatic synthesis of 3' Amino-3'-deoxynucleoside, a building block for oligonucleotide N3'? P5' phosphoramidate.

PP-419

MICROWAVE ASSISTED SYNTHESIS OF SOME NOVEL PYRAZOLONE DERIVATIVES

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ABSTRACT

Pyrazolone derivatives have attracted intense interest in recent years due to their different pharmacological properties which depend upon the pattern of substitution. They have been widely studied for their importance as antipyretics, analgesic and anti-inflammatory agents. The aim of the present paper is to show that application of microwave irradiation decreased the required time and is applied in the organic synthesis as inexpensive, non-corrosive and environment friendly technique. Synthesis of some novel pyrazolone derivatives can be successfully done with purity under microwave irradiation . As in microwave-induced organic reaction ethyl a-(4-chloro-2-methyl phenyl azo) acetoacetate (0.01 mol) and acid hydrazides of malon anilic series (0.01 mol) were taken into a 250 ml conical flask and is subjected to microwave irradiation for 60-110 seconds. These newly synthesized compounds were characterized by elemental, IR and NMR analysis.

PP-420

In vitro anti - fungal activity of essential oils of some plants of North east India

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ABSTRACT

Plant essential oils are used as an anti fungal agent since a long time and we report here the evaluation of six plant essential Oils against the anti dermatophytic and anti - Candida activities against six dermatophytic species. The selected essential oils were screened against- *Trychophyton rubrum, Trychophyton mentagrophytes, Trychophyton ajelloi, Microsporeum gypseum, Microsporeum fulvum* and *Microsporum canis.* The antifungal activities of essential oils were evaluated by the agar-well diffusion method (1). The MICs of the active essential oils were tested using two fold agar dilution methods at concentrations ranging from 0.2 to 10.6 mg/ml (2). All the extracted oils exhibited considerable anti-dermatophytic activities against one or more strains.

PP-421

Plasmodium falciparum Transketolase and Purine Nucleoside Phosphorylase: Potential Drug Targets

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ABSTRACT

Malaria is one of the leading causes of morbidity and mortality in the Tropics. Due to emergence of drug resistance in the parasite against commonly used drugs, an urgent need exists to identify new drug targets and develop new pharmacophores with unique structures and modes of action. Targeting the parasite's metabolic pathways that lead to the formation of functional and structural components of the parasite can be a good strategy for new anti-malarial development. The pentose phosphate pathway (PPP) is an important metabolic pathway for yielding reducing power in the form of NADPH and production of pentose sugar needed for nucleic acid synthesis. Transketolase, the key enzyme of nonoxidative arm of PPP, plays a vital role in the survival/replication of the malarial parasite. *Plasmodium* parasites are auxotrophs for purine bases and use hypoxanthine for purine salvage pathway. Purine nucleoside phosphorylase has dual cellular functions in purine salvage and polyamine metabolism. The *Plasmodium falciparum* obtains hypoxanthine either from erythrocytes or itself synthesizes by sequential action of adenosine deaminase (PfADA) and purine nucleoside phosphorylase (PfPNP). This hypoxanthine in parasite is first converted to inosine monophosphate (IMP) by the enzyme hypoxanthine-guanine-xanthine phosphoribosyl-transferase (PfHGXPRT) which is subsequently used as a precursor for synthesis of purines. 5'-methylthioadenosine (MTA), a

product of polyamine metabolism has been reported to be strong inhibitor of spermine synthase, sperimidine synthase and ornithine decarboxylase. Due to its involvement in two key metabolic processes, PfPNP in *Plasmodium* is considered as an important drug target in malaria. PfTK and PfPNP were cloned, expressed and purified from bacterial cell system. The recombinant PfTk catalyzed the oxidation of donor substrates, fructose-6-phosphate (F6P) and hydroxypyruvate (HP) and p-Hydroxyphenylpyruvate showed potent inhibition of PfTk, when hydroxypyruvate was used as a substrate. The native PfTk a hexamer with subunit molecular weight of 70 kDa, upon treatment with low concentrations of guanidine hydrochloride (GdmCl) dissociated into functionally active dimers. This protein was localized in the cytosol and nucleus of the parasite. An integrated pharmacophore based virtual screening using CDRI small molecule database against PfTk lead to identification of novel and chemically diverse inhibitors. The kinetic properties of PfPNP also showed significant difference as compared to host. PfPNP accepts inosine and guanosine as substrate but not adenosine. The single tryptophan residue residing in conserved region of transition loop is present in purine nucleoside phosphorylases throughout *Plasmodium* genus. Chemical modification studies suggested that single tryptophan is essential for its activity but not for substrate binding. The observed differences in the kinetic properties of parasitic enzymes as compared to the host enzyme may facilitate designing of novel inhibitors of PfTk and PfPNP with potential anti-malarial activity.

PP-422

A novel ligand free Pd-catalyzed cascade reaction: An access to the highly diverse Isoquinolin-1(2*H*)-one derivatives via isocyanide and Ugi-MCR synthesized amide precursors

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ABSTRACT

A novel ligand-free palladium catalyzed cascade reaction for the synthesis of highly diverse isoquinolin-1(2*H*)-one derivatives [1] from isocyanide and amide precursors synthesized by Ugi-MCR has been developed. A broad variety of acids, amines and isocyanides were used as starting materials for Ugi-MCR leading to various amide precursors, which in turn provided entry into diverse isoquinolin-1(2*H*)-one derivatives.[2-4] The reaction proceeds through tandem isocyanide insertion with intramolecular cyclization followed by Mazurciewitcz-Ganesan type sequence to provide isoquinoline-1(2*H*)-one derivatives in moderate to good yield.[5,6]

PP-423

Synthesis of ß-carboline derivates and their bioevaluation as antileishmanial agents

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ABSTRACT

The Leishmaniases are a spectrum of neglected parasitic diseases caused by different species of the genus *Leishmania* protozoan, which is transmitted to humans by the bite of female phlebotomine sand fly. The disease is endemic in 88 countries, and there are 500 000 new cases of its visceral form each year, leading to 50 000 deaths. [1] Natural and synthetic ß-carbolines and tetrahydro-ß-carbolines alkaloids are well-known compounds that possess a variety of biological properties. In 1998, a tetrahydro-ß-carboline alkaloid buchtienin was isolated from *Kopsia griffithii* and found to have good antileishmanial activity ($0.30 < IC_{50} < 1.56$ mg/ml) against *L. donovani*. [2] Later, annomontine, a pyrimidine-ß-carboline alkaloid, isolated from the bark of a Brazilian tree *Annona foetida*, [3] was also reported to be active against leishmania.

As part of our continuing efforts towards the design and synthesis of novel nitrogen heterocylces anti-infective agents, our group has identified some synthetic analogues of ß-carboline potent against leishmania.[4] Herein, we propose to synthesize some natural product based novel ß-carboline derivatives inorder to discover a new class of antileishmanial agents.

PP-424

Access to indole- and pyrrole-fused diketopiperazines via tandem Ugi-4CR / intramolecular cyclization and its regioselective ring opening by intermolecular transamidation

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ABSTRACT

Among the various bioactive heterocyclic molecules, Diketopiperazines (DKPs) constitute an unique class of compounds as a "privileged" scaffold present in many natural products and are responsible for a wide range of biological activities[1] as antitumor, antiviral, antifungal, antibacterial, antihyperglycemic agents, GABA-ergic and oxytocin receptors, etc. Several natural products as Gliotoxin,[2] Glionitrin B,[3] Spirotryprostatin A,[4]Demethoxyfumitremorgine C,[5] WIN 64821 and WIN 6474[6] contains hetero-fused DKP fragments. Additionally *1H*-indole-2-carboxamide and *1H*-pyrrole-2-carboxamide templates are present in natural products as well as in numerous biologically active compounds associated with wide range of biological activity. In the light of above fact, herein we report an efficient approach for the synthesis of indole- and pyrrole-fused diketopiperazines has been developed. This protocol involves the Ugi four-component reaction (U-4CR) followed by an intramolecular cyclization of the Ugi products at room temperature to afford the desired products in good to excellent yields. In addition, it is interesting to report the subsequent regioselective ring opening of diketopiperazine unit occur via an intermolecular transamidation reaction under mild condition, resulting in the formation of highly functionalized indole-2-carboxamides and pyrrole-2-carboxamides.

PP-425

N-(3-(5R-[1,2,4]triazino[5,6-b]indol-3-ylthio)alkyl-7-chloroquinoline-4-amine: A new series of Antileishmanial Agents

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ABSTRACT:

Leishmaniasis, one of the most significant of the neglected tropical diseases, with 350 million people in 88 countries worldwide living at risk of developing one of the many forms of the disease, caused by infection with one of several different species of protozoan parasites of the genus *Leishmania*, which maintain their life cycle through transmission between an insect (sandfly) and a mammalian host. Treatment of VL relies on specific anti-leishmanial drugs and the aggressive management of any concomitant bacterial or parasitic infections, anaemia, hypovolemia and malnutrition and medicinal science still looking for less toxic and cheaper medicines [1]. We have synthesized a novel series with the aim of generating new antileishmanial against *L. donovani* and interestingly some of these compounds have shown good antileishmanial *in vitro* activity. Triazino indole unit is natural pharmacophore, its derivatives cover a broad spectrum of antibacterial, antifungal, antiparasitic and anticancer activities [2] while quinoline is a good pharmacophore [3].

PP-426

Exploration of the Activity of Norfloxacin Derivatives against Methicillin, Vancomycin and Gentamycin-Resistant strain of *Staphylococcus aureus*

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ABSTRACT:

During 1980s, the introduction of norfloxacin the first fluoroquinolone, and later on, the discovery of other fluoroquinolones like ciproploxacin, sparfloxacin and trovafloxacin have changed the landscape of antibacterial chemotherapy.[1,2] Over the past several years, community-associated methicillin-resistant *Staphylococcus aureus* (MRSA) strains have been involved in an increasing number of serious infections not originating in the hospital setting. [3] The development of bacterial resistance to the currently available antibacterial agents is a growing global health problem.[4] Therefore, to develop new effective antibacterials that may work out in increasing the efficacy against resistant bacteria, we have synthesize some new analogues of certain novel norfloxacin derivatives with an additional functional moiety ethyl-4-(trifluoromethyl)benzene at N-1 position (to provide extra hydrogen bonding capacities with the DNA gyrase) and evaluated their antibacterial activity against methicillin-resistant *S. aureus* (MRSA), methicillin-resistant, vancomycin-resistant *S. aureus* (VRSA) and gentamycin-resistant *S. aureus* (GRSA).

PP-427

Synthesis of Perspicamide A and Related Analogues: Their Bio-evaluation as Potent Antileishmanial Agents

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ABSTRACT

Leishmaniasis, one of the leading cause of death by parasitic protozoa of the genus Leishmania. Among them visceral leishmaniasis (VL) is most severe form called Kala-azar or black fever, can have a fatality rate as high as 100% within two years if left untreated . In this perspective, Perspicamide A & B were first isolated from the Australian ascidian *Botrylloides persipicuum* in 2005 by Matthew J. McKay *et a1*[1]. Since long time our interest to synthesized potential bioactive molecules for anti-infective diseases[2], We achieved the first synthesis of Perspicamide A and related diverse analogues. The synthesized molecules were tested for antileishmanial activity against *Leishmania donovanii* strain consequently few of the synthesized analogues were found more active and safe compare to the standard drug Miltefosine (IC_{50} 12.4, Selectivty index(SI) 4.41).

PP-428

ISOLATION AND IDENTIFICATION OF *β*-HEMATIN INHIBITORS FROM *FLACOURTIA INDICA* AS PROMISING ANTIPLASMODIAL AGENTS

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ABSTRACT

Malaria is a devastating infectious disease, causing great suffering and loss of human life [1]. Out of the five malaria species infecting humans, *Plasmodium falciparum* is responsible for the majority of deaths [2]. The resistance of *P. falciparum* to chloroquine and other antimalarial drugs [3, 4] has created an urgent need for the development of new drugs that are safe and effective for the treatment of malaria. Natural products have played a pivotal role in drug discovery and the development of malaria chemotherapy [5-7], and will continue to be a source of new chemical entities.

As part of a drug discovery programme from Indian medicinal plants, ethanolic extract (A001) of the leaves and twigs of *Flacourtia indica* (Burm.f.) Merr., was purified to give a new phenolic glycoside, 2-(2-benzoyl-*β*-D-glucopyranosyloxy)-7-(1*a*, 2*a*, 6*a*-trihydroxy-3-oxocyclohex-4-enoyl)-5-hydroxybenzyl alcohol (**1**) together with poliothrysoside (**2**), catechin-[5,6-*e*]-4*β*-(3,4-dihydroxyphenyl)dihydro-2(3*H*)-pyranone (**3**), 2-(6-benzoyl-*β*-D-glucopyranosyloxy)-7-(1*a*, 2*a*, 6*a*-trihydroxy-3-oxocyclohex-4-enoyl)-5-hydroxybenzyl alcohol (**4**), chrysoeriol-7-O-*β*-D-glucopyranoside (**5**), and mururin A (**6**). They were subjected to *in vitro* antimalarial assay. **6** was found to be the most active compound, which significantly inhibited the *in vitro* growth of both a chloroquine-sensitive (3D7) and a chloroquine-resistant (K1) strain of *Plasmodium falciparum* with an IC_{50} of 1.2±0.1 μM and 1.3±0.1 μM, respectively. Further mechanistic study showed that it forms a complex with hematin and inhibits *β*-hematin formation, suggesting that this compound act on a heme polymerization target.

PP-429

Facile and Greener Protocol for the Synthesis of 1, 2, 4-Triazole Based 1, 4-Diarylquinoline Derivatives

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ABSTRACT

Quinolines and there derivatives have played crucial role in the development of heterocyclic chemistry and have been used extensively as an important pharmacophores and synthones in the field of medicinal chemistry. Many classes of chemotherapeutic agents are having quinoline and triazoles as core nuclei and these are currently in clinical use. There are numerous quinoline containing drugs have been used in the treatment of various diseases viz. antitumor, antibacterial, anti-fungal, antimalarial and anticancer activities.[1] In view of the pharmacological importance of quinolines, here we have synthesized novel heterocyclic frameworks containing quinoline and 1, 2, 4triazole as pharmacophores with hope to obtain the compounds with intensified bioactivities. The traditional methods available for the synthesis of quinolines are associated with either organic solvents or hazardous volatile organic compounds. In this regard, it was thought worthwhile to investigate an efficient synthetic route for this potentially active compounds using PEG-400 under environmentally benign condition. The developed protocol affords correspond to synthesize 1, 4-diarylquinolines by green aspect avoiding toxic catalysts and solvents in good to excellent yield.

PP-430

Identification and Comparison of Bioactive Compounds in different plant parts of Piper *nigrum* by Direct Analysis in Real Time-Mass Spectrometry

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ABSTRACT

Plants belonging to the genus piper are reputed in the Indian ayurvedic system of medicine for their medicinal properties. Piper *nigrum* L. is a traditional medicine widely used in India for illnesses such as constipation, diarrhoea, earache, gangrene, heart disease, hernia, hoarseness, indigestion, insect bites, insomnia, joint pain, liver problems, lung disease, oral abscesses, sunburn, tooth decay and toothaches [1]. In the present study, DART-MS, a recently introduced ambient analytical technique, has been found as a rapid analytical tool without any sample preparation for the identification and comparative study of bioactive compounds in different plant part of Piper *nigrum* such as fruit, root and leaves. The volatile aroma constituents like monoterpenoids and sesquiterpenoids, along with the pungent piperamides were detected using DART-MS. Aliphatic hydrocarbons and phenolic compounds were also identified through exact mass measurements using DART-HRMS. DART-MS[2,3] is a simple, rapid, high-throughput tool for qualitative confirmation of chemical identity, quantification of constituents and metabolomic fingerprinting and profiling. The method is accepted widely in natural product research, especially in food quality control and in food authentication. DART-HRMS can give accurate molecular weight, so that a single molecular formula can be deduced. The present work is the first report of the application of DART in the chemical analysis of Piper *nigrum.*

PP-431

Identification of Gender Specific Discrimination in *Tinospora cordifolia* Stem using LC-QTOF-HRMS Technique

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ABSTRACT

Tinospora cordifolia plant is known for its many medicinal properties and stem of *Tinospora cordifolia* plant is mainly used in ayurvedic preparations.[1] It has been used for several centuries in the Indian system of medicine for the treatment of jaundice, diabetes, skin diseases and anaemia.[2] The active principles of *Tinospora cordifolia* were found to possess anticomplementary and immunomodulatory activities.[3] The different class of biologically active compounds such as alkaloids, diterpenoids lactones, glycosides, steroids, phenolics, sesquiterpenoids, polysaccharides and other aliphatic compounds are reported in the Tinospora cordifolia plant. Quadrupole time of flight mass spectrometric technique has been applied for the first time for the male and female discrimination of *Tinospora cordifolia* plant. The results show that the plant type male and female could be easily differentiated using LC-QTOF-MS data and chemical profiling clearly indicate the presence of characteristic compound in *Tinospora cordifolia* plant under investigation. Some medicinally important compounds namely Jatrorrhizine, Magnoflorine, Tembetarine, Tetrahydropalmatine, Columbin, and ß- Sitosterol are found in both male and female plant by their molecular formula and exact mass measurement.

PP-432

DART MS Based Chemical Profiling for Therapeutic Potential of *Piper betle* Linn. Landraces

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ABSTRACT

Piper betle Linn. (PB) leaves are traditionally used as a folk medicine in India. *Piper betle* is a Asiatic plant having cultural and medicinal uses. It belongs to family Piperaceae and native of tropics though it is also cultivated in subtropical areas. Indian system of medicine Ayurveda recognized the importance of PB. It is known to have digestive, carminative, anti-inflammatory, cardiotonic ,anti-fertility[1] , anti-amoebic , anti-oxidant[2] , photoprotective , larvicidal , anti-allergic , anti-fungal , radioprotective , hepatoprotective , anti-diabetic, wound healing properties, antimicrobial activity[3].Twenty one PB landraces were analyzed using Direct Analysis in Real Time (DART) mass spectral technique and evaluated on the basis of molecules detected in leaves. Clustering of landraces based on three well known biologically active phenols (m/z 151,165,193) showed two broad groups with high suggesting differences in their therapeutic potential. Findings of this study could be useful in rapid screening of the landraces for determining their medicinal potential.

PP-433

Development and validation of a stability indicating UPLC assay method for determination of chlorhexidine gluconate and lidocaine hydrochloride in throat spray

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ABSTRACT

The objective of the current study was to developed simple, precise and accurate gradient reversed-phase stability indicating UPLC assay method and validated for determination of chlorhexidine gluconate and lidocaine hydrochloride in throat spray. Isocratic RP-UPLC separation was achieved on a Waters Acquity BEH C18, 2.4 x 50mm, 1.7µ column. The flow rate of the mobile phase was adjusted to 0.3 ml/min and the injection volume was 4µl partial loop with needle overfill. Detection was performed at 215nm using photo-diode array detector. The drug was subjected to oxidation, hydrolysis, photolysis and heat to apply stress condition. The method was validated for specificity, linearity, precision, accuracy, robustness and solution stability. The method was linear in the drug concentration range from 0.040-0.160 mg/ml with with correlation coefficient 0.9997 for Chlorhexidine gluconate and 0.016-0.064 mg/ml with correlation coefficient 0.9994 for Lidocaine hydrochloride. The precision (RSD) amongst six-sample preparation was 0.42 % for repeatability and the intermediate precision (RSD) amongst six-sample preparation was 0.53 % for Chlorhexidine gluconate. The precision (RSD) amongst six-sample preparation was 0.33 % for repeatability and the intermediate precision (RSD) amongst six-sample preparation was 0.33 % for Lidocaine hydrochloride. The mean recovery for Chlorhexidine gluconate was 98.6-99.80 % and for Lidocaine hydrochloride 99.17-99.52 %. Degradation products produced as a result of stress studies did not interfere with detection of chlorhexidine gluconate and lidocaine hydrochloride and the assay can thus be considered stability indicating.

PP-434

Hydroarylation of arenes with styrenes using Montmorillonite K-10 as an efficient, selective, and recyclable catalyst

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ABSTRACT

Catalytic functionalization of arenes and heteroarenes has considerable importance in the pharmaceutical, agrochemical, fine and bulk chemical industry. It is one of the most important C-C bond formation methodology. Traditionally, acylation, alkylation, nitration, and halogenations of arenes were carried out by Friedel Crafts reactions for such transformations. However, these methods have several limitations like the use of stoichiometric amount of Lewis acids, drastic reaction

conditions, lower selectivity and large amount of salt formation. Recently, several papers report organometallic catalysts [1] as an efficient tool for the environmentally benign C-H functionalisation like Freidel-Crafts hydroarylation of the arenes. The products diarylalkanes which has great importance in various valuable biological active compounds and pharmaceutics.
Hydroarylation of styrene and its derivatives with arenes and heteroarenes was studied using Montmorillonite K-10 as an efficient, environmentally benign, economical, greener, and recyclable catalyst. The reaction gives 1,1-diarylalkanes with a very excellent selectivity and excellent yields in short time with greater substrate compatibility. Solid acid Montmorillonite K-10 catalyst was thoroughly characterized with different techniques. Notable advantages offered by this metal-free reaction system are the use of Montmorillonite K-10 as a heterogeneous recyclable catalyst, simple workup procedures; higher yields of the desired products and greater substrate compatibility making this approach an important supplement to the existing methods.

PP-435

Health and wellness by natural products and Neutraceuticals

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ABSTRACT

Nutraceuticals are referred by different terminologies like functional foods, fusion foods, dietary supplements, designer foods etc. The term 'functional foods' refers to processed foods containing ingredients that aid specific bodily functions in addition to being nutritious. Nutraceuticals are found in a mosaic of products such as the food industry, the herbal and dietary supplements, the pharmaceutical industry such as tablets, soft gels, capsules etc.
A nutraceutical is a product isolated or purified from foods, generally sold in powders, pills, and other medicinal forms not usually associated with food, and demonstrated to have a physiological benefit or provide protection against chronic disease." The term nutraceutical was originally defined by Dr. Stephen L. DeFelice, founder and chairman of the Foundation of Innovation Medicine (FIM), Crawford, New Jersey. **Nutraceuticals** are formulations of high quality, **all natural functional food products** for enhanced health and wellness. Our **antioxidants, body detoxifiers,** broad spectrum **micronutrients, macronutrients** and **joint pain relief** products. Nutraceuticals are used as conventional foods or as sole items of a meal or diet. Dietary components play beneficial roles beyond basic nutrition, leading to the development of the functional food concept and nutraceuticals. A functional food for one consumer can act as a nutraceutical for another consumer. Examples of nutraceuticals include fortified dairy products (e.g., milk) and citrus fruits (e.g., orange juice). Astaxanthin is a red colored carotenoid pigment that naturally occurs in most marine crustaceans and some species of fish. Astaxanthin has an antioxidant action up to 500 times that of vitamin E, which has led some experts to term it as "Super Vitamin E". Astaxanthin is the most stable antioxidant. Antioxidants: resveratrol from red grape products; flavonoids inside citrus, tea, wine, and dark chocolate foods; anthocyanins found in berries, Vitamin C . Reducing hypercholesterolemia soluble dietary fiber products, such as psyllium seed husk. Cancer prevention: broccoli (sulforaphane) fiddleheads (Matteuccia Struthiopteus). Improved arterial health: soy or clover (isoflavonoids). Lowered risk of cardiovascular disease: alpha-linolenic acid from flax or chia seeds, Omega 3 fatty acids in fish oil. B-Sistosterol, a plant phytosterol reduces blood levels of cholesterol, also used in the treatment of benign prostrate hypertrophy, tandem Xanthoma. Borage oil, an important source of linolenic acid which can improve overall health. Some of the nutraceuticals are Citrus Bioflavinoid, Cordcep Sinesis, Flax seed oil, Spirullina, dry fruits like fig, apricot, dry cherries etc., which are the natural products produces health and wellness to the humans.

PP-436

GENETICALLY ENGINEERED PROBIOTICS AS PHARMA FOODS

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ABSTRACT

The intestinal microbiota is a key component of both the metabolism and immunity of humans and animals. These can be helpful in healthcare, especially for the management of digestive diseases and food-borne illnesses. Through genetic engineering it became possible to fully express biologically active copies of such powerful molecules from food and commensal bacteria. Genetically engineered probiotics can be used to treat inflammatory bowel diseases such as Crohn's disease and ulcerative colitis, as well as other disorders resulting from an overactive immune system. In a recent research, scientists deleted a gene from the bacterium *Lactobacillus acidophilus,* which is responsible for increasing inflammation, a

defining characteristic of Crohn's disease and ulcerative colitis. But the unaltered form of the bacterium also triggered production of a beneficial immune molecule, IL-10m, which helps to regulate the immune system. Thus, the goal of engineering the microbes is to deliver the beneficial effects without the harmful ones. Besides, the future of genetically modified probiotics is in food additives to control the release of human growth factors by the modified bacteria to fight against injury and inflammation in the gut *e.g.* the use of a plant sugar called xylan to stimulate the genetically modified human gut probiotic bacterium *Bacteroides ovatus* to produce specific proteins that can repair damaged cells and dampen down the immune system in the intestine that causes inflammation and disease. Administration of xylan with the genetically engineered probiotic bacteria resulted in a significant improvement of colitis, reduced weight loss, improved stool consistency, reduced rectal bleeding and accelerated healing of damaged colonic cells. GM probiotics posses potential in clinical applications e.g. delivery of antigens for vaccines and thus are more readily accepted. This would provide a safer method of vaccination than the use of attenuated pathogens e.g. GM, *Lactococcus lactis*, produces IL-10 in the mouse intestine. This may provide new treatment strategies for inflammatory bowel disease, and similar applications may be useful for other diseases.

PP-437

Synthesis of Silicon Materials from Rice Husk Ash as a Carboneous Waste material

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ABSTRACT

Rice husks (RH) from rice grains are removed as waste while refining of rice that composed of cellulose, hemicelluloses, lignin and silica (about 65-70%) and acts as viable raw material for production of silica gels and powders. 20 million tons of RHA waste is produced annually in India which causes an environmental problem due to air and water pollution, so, not unusual that this cheap source of silica may be of interest for numerous industrial uses like amorphous RH derived silica provides a path way for production materials such as silicon ,Zeolite, concrete and cements surfactant. Ash of RH (rice husk) contains silica source for Zeolite synthesis due to its high ash content (13 to 29 wt% depending on the variety, climate and geographic location). Silica in husk is in hydrated amorphous form, either opal or silica gel. Silica powder with approximately 98% purity was extracted from rice husk (RH), converted to a sodium silicate solution, and used as a silica source for the synthesis of low silica.

PP-438

Coal depolymerizing activity by lignolytic enzymes

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ABSTRACT

Present chemical industry is based on oil reserves which are depleting. One possible alternative is the use of coal for the generation of chemicals. In order to use coal for generation of chemicals, high molecular weight coal fractions should be converted into low molecular weight coal fractions. Since coal has chemical composition similar to lignin, lignolytic micro-organisms and lignolytic enzymes are expected to depolymerize coal. Keeping these points in view work has been initiated on depolymerisation studies on coal using humic acid as a model of coal and lignolytic fungi namely *Polyporus biennis* MTCC-1176, *Pestalotia bicolor* MTCC-372, *Heterobasidion annosum* MTCC-146, *Pleurotus ostreatus* MTCC-142, *Gloephyllum striatum* MTCC-1117, *Loweporus lividus* MTCC-1178, *Pleurotus sajor caju* MTCC-141, *Fomes durissimus* MTCC-1173, *Hexagona tenuis* MTCC-1119, *Gloephyllum sepiarium* MTCC-1170, *Pycnoporus sanguineus* MTCC-137, *Xylaria polymorpha* MTCC-1100, *Trametes hirsuta* MTCC-1171, *Lenzites betulina* MTCC-1183, *Phellinus linteus* MTCC-1175 and *Daedalea flavida* MTCC-145. An extensive studies on depolymerisation of coal by indigenous lignolytic fungi and their lignolytic enzymes is being done with a view to identify efficient micro-organisms and efficient enzymes.

PP-439

Characterization and Production of pectinolytic enzymes by *Xanthomonas axonopodis citri* isolated from various sources

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ABSTRACT

Xanthomonas are yellow pigmented motile, aerobic rods mostly pathogenic to cultivated and wild plants. Species of *Xanthomonas* causes some of the most serious diseases in plants. Seventy eight *Xanthomonas axonopodis citri(Xac)* strains were isolated from citrus rinds, leaves and stem. *Xac* produces extracellular cell wall degrading enzyme that degrade the pectic layers of plant cell wall and provide entry in the host plants. Pectinesterase (PE), Polygalacturonic acid trans-eliminase ((PATE), Pectin methyl esterases (PME), Pectin lyases(PL) and Pectate lyases(PAL) are produced on pectin or pectic acid based medium by all *Xac* strains screened. Pectinesterase production was found in the culture containing pectin as the substrate rather than polygalacturonic acid or glucose. PE, PAL and PME activity was found in higher concentration than PL and PATE *Xac* isolated from leaves. *Xac* isolated from stem showed only PE and PATE activity. PME, PL and PATE enzyme were synthesized by *Xac* isolated from citrus rind

PP-440

Synthesis of benzimidazolyl pyrazolines derived from paracetamol hydrazide and isoniazide as potential antimicrobial agents.

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ABSTRACT:

In the present paper, pyrazoles, paracetamol hydrazide and isoniazide were attached to benzimidazolyl chalcones to get desired compounds *N*-(4-(2-(3-(*1H*-benzo[*d*]imidazol-2-yl)-5-(aryl)-4,5-dihydro-*1H*-pyrazol-1-yl)-2-oxoethoxy)phenyl) acetamides **6a-p** and 3-(*1H*-benzo[*d*]imidazol-2-yl)-5-(aryl)-4,5-dihydro-*1H*-pyrazol-1-yl)(pyridin-4-yl)methanones (**8a-p**) respectively. Benzimidazolyl chalcones were synthesized by Claisen-Schmidt condensation. The structures of newly synthesized compounds were elucidated by IR, ^{1}H NMR, ^{13}C NMR, and mass spectral analysis. All bio-active molecules were tested for their *in vitro* antibacterial activity against the representative panel of Gram-positive (*Staphylococcus aureus*, *Streptococcus pyogenes*) and Gram-negative (*Escherichia coli*, *Pseudomonas aeruginosa*) bacteria by serial broth dilution method. Same compounds were also tested for their inhibitory action against three strains of fungi (*Candida albicans*, *Aspergillus niger*, *Aspergillus clavatus*) and have exhibited moderate to excellent growth of inhibition against bacteria and fungi.

PP-441

The asymmetric Nitroaldol (Henry) reaction of Trifluoromethyl Ketones catalyzed by new Cu(I) chiral catalyst

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ABSTRACT

The asymmetric nitroaldol reaction is a powerful synthetic tool for the stereoselective C-C bond forming reaction because the resultant *ß*-hydroxynitroalkanes are important building blocks for the preparation of *ß*-amino alcohol derivatives, a-hydroxycarboxylic acid and *ß*-receptors [1,2].On the other hand, due to wide range of applications oforganofluorine compounds, this is an important field of research[3].Among them, trifluoromethyl-substituted molecules constitute an interesting class of compounds because of their relevant properties[4] for the pharmaceuticals and agrochemicals.So, the asymmetric synthesis of (*R*)-trifluoromethyl tetra substituted carbons has concerned much attention, mainly because of the emergence of drugs such as Efavirenz (anti-HIV).Herein we describe the direct catalytic enantioselectivenitroaldol (Henry) reaction of simple α-trifluoromethyl ketones with various nitroalkanes with chiral Cu(I) bromide salt complex. The resulting α-trifluoromethyl tertiary Nitroaldol products were obtained in moderate to high yields (up to 90%) and enantioselectivities (up to 99% ee) with 2.5 mol% catalysts loading at RT in 25h.

PP-442

Asymmetric Cyano-ethoxycarbonylation Reaction of Aldehydes Catalyzed by Ti^{IV} Macrocyclic Complex: A Protocol for the synthesis of ß- Blocker and a_1-Adrenergic Receptor Agonist

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ABSTRACT

Asymmetric cyano-ethoxycarbonylation reaction of aldehydes is an attractive strategy for the synthesis of ß-Blocker and a_1-Adrenergic Receptor Agonist.[1,2]Chiral macrocyclic Ti(IV) salen complexes Ti-1a, used as efficient catalysts in asymmetric cyano-ethoxycarbonylation of aldehydes. The Ti (IV) catalysts demonstrated excellent performance (product yields and ees up to 99%) using ethyl cyanoformate as source of cyanide with low catalyst loading 0.5 mol% (lowest loading with best of our knowledge). The Ti(IV)macrocyclicsalen complex Ti-**1a** retained its performance at multi-gram level and was conveniently recycled for a number of times. The product obtained was straightforwardly transformed to the pharmaceutically important chiral drugs (R)-Proethalol (ß-Blocker) and (R)-Phenylephrine (a_1-Adrenergic Receptor Agonist) in good yield. To understand the mechanism of the catalytic reaction, the kinetic investigation was carried out with various concentrations of the catalyst, ethyl cyanoformate and benzaldehyde as the representative substrate. The reaction of benzaldehyde was first order with respect to the concentration of the catalyst and the ethyl cyanoformate but did not depend on the initial concentration of the substrate. A possible mechanism of the cyano-ethoxycarbonylation reaction isproposed.

PP-443

Synthesis and In-vitro activity of 4-Amino substituted Quinolines as Antimalarial agents

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ABSTRACT

Malaria is one of the major problems of many tropical and subtropical countries in the world. There are a several classes of antimalarial drugs, which inhibit different stages of the malaria parasite, but as the parasites rapidly develop permanent resistance against the different subclasses, there is a great urge to develop new and effective drugs. Designing hybrid drugs with multiple effects is a common strategy in today's search for new treatment of malaria. CQ and other structurally related antimalarials exert their effect by binding to heme molecules released from the hemoglobin that is digested by malaria parasites on the other hand pyrimidine derivatives, are potent DHFR inhibitors have been reported to possess antimalarial activity. Hybrid drug approach involves the incorporation of two drug pharmacophore in one single molecule with attention of dual drug action.
Synthesis of antimalarials is based on novel pharmacophores. We have synthesized 4-Aminoquinolino-pyrimidines to overcome the resistance against chloroquine and tested for ß-hematin inhibitory activities. Synthesis and activity of 4-aminoquinolino-pyrimidines will be present in the conference.

PP-444

Design and synthesis of novel spiro quinazolinone-based heterocycles as Potential Hypolipidemic agents

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ABSTRACT

Dyslipidemia and hypertension are among the major risk factors of the development of atherosclerotic condition, are interrelated [1]. Statins and fibrate class of drugs are the most widely used candidates for treatment of dyslipidemia [2]. However, due to side effects, high doses and safety issue regarding these, there is a constant need for a different class of potent compounds to treat dyslipidemia without severe side effects [3]. Quinazolinone and indole group is a vital part of a natural product and a number of compounds with a wide range of biological activities. Notably, several biologically active molecules and natural products contain spirooxyindole ring system [4,5]. These pharmacophores are also found in a variety of antiobesity agents. To circumvent the problem of drug resistance, design of new drugs based on new strategy is highly prioritised. Therefore, the development of quinazolinone analogues based on hybridization approach may lead to compounds with moderate to good hyperlipidemic profile.

PP-445

X-ray crystallographic study and DFT calculations of 3,4,6,7-tetrahydro-3,3,6,6-tetramethyl-2H xanthenes 1,8(5H,9H) dione

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ABSTRACT

In the present study xanthene dione, a coumarin derivative, was synthesized and studied by X-ray crystallography and theoretical methods. Xanthene dione is a biologically active molecule that shows good antibacterial and antifungal properties and is an optically active compound. The molecule crystallizes in triclinic crystal system with P-1 space group. Density functional theory (DFT) calculations were performed at Becke's three-parameter functional and Lee–Yang–Parr functional (B-3LYP) level of calculation and the 6-31G++ basis set was used for ground state geometry optimization. The *xyz* coordinates obtained via X-ray crystallography have been taken for the geometry optimization in DFT. A close comparison of the selected bond lengths and bond angles of the crystal structure and theoretically optimized structure by DFT have shown only marginal difference. The DFT study of electron surface potential (ESP), showed a large intramolecular charge transfer efficiency of the molecule indicating optical active of xanthene dione

PP-446

Polyalthia longifolia var. pendula as potential lipid lowering agent: Discovery of a new class of HMG-CoA reductase inhibitor

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ABSTRACT

Atherosclerosis is the major cause of heart disease, stroke and death in developed and developing countries. Elevated lipid levels continue to be the primary risk factor for this disease. Epidemiological studies have shown that dyslipidemia and coagulation disturbances are among the most significant risk factors of the development of atherosclerotic condition. Current pharmacological treatments include use of statins a class of HMG-CoA reductase inhibitors. Undesirable side effects of statins lead to a constant need for a different class of potent compounds to treat dyslipidemia without severe side effects.
Bioassay guided fractionation of the ethanolic extract of ***Polyalthia longifolia*** var. pendula, led to the discovery of the clerodane diterpene, 16a-hydroxycleroda-3, 13 (14) Z-dien-15, 16-olide (1), as a new structural class of HMG-CoA reductase inhibitor as a potential antidyslipidemic agent.

PP-447

Evaluation of Phytoconstituents and Invitro alpha amylase inhibitory effect of *Costus speciosus* L. in the Management of Diabetes

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ABSTRACT

Diabetes is a disorder of carbohydrate metabolism and alpha-amylase inhibitors are often an effective strategy to control postprandial hyperglycemia via the control of starch breakdown. *Costus speciosus* L. is a medicinal plant widely distributed in India and used in ancient Ayurveda and traditional medicinal practices. The present study was carried out to evaluate the phytoconstituents from leaves and rhizomes of this plant for antioxidant properties. The total phenolic content of the extract was determined by TLC and estimated spectrophotometrically by using Gallic acid equivalents. Certain phenolic compounds such as umbelliferone, aureusidin-4-glucoside were detected by technique like TLC and absorption spectra. Presence of tannins ,flavanoids, glycosides and saponins was also detected by qualitative tests [1]. The extracts were also evaluated for antioxidant enzymes Catalase and Peroxidase. The total flavanoid content was determined by quercetin equivalent. The extracts were further evaluated for their effect on alpha-amylase ,which is an important enzyme in carbohydrate metabolism. The extract from leaves showed 75% inbition of alpha amylase activity and the extract from roots showed 90% inhibition when compared with commercial inhibitor acarbose. Our results showed that the plant is rich in phytoconstituents, antioxidant enzymes due to which it could be considered as a potential candidate in the management of diabetes.

PP-448
A STABILITY INDICATING HPLC METHOD FOR THE DETERMINATION OF METFORMIN USING ECOFRIENDLY SOLVENT AS MOBILE PHASE

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ABSTRACT
The present paper describes the use of Solvent-X (Propylene Carbonate: Methanol, 60:40) as a mobile phase component in place of Acetonitrile (ACN). A need to replace ACN with a new environmental friendly solvent is increasingly gaining importance because ACN is ranked by the EPA as a hazardous solvent. The waste has to be incinerated and the NO_2 released is partly responsible for acid rain which has an ill effect on human health. Solvent-X has numerous advantages over ACN with respect to dipole moment, dielectric constant, biodegradability, clinical toxicity etc. Besides showing similar selectivity characteristics, Solvent-X has certain significant advantages over ACN.
The objective of the current study was to develop a simple, economic, and time-efficient stability-indicating, reversed-phase high-performance liquid chromatographic method for Metformin HCl in the presence of both, related impurities: a.) Cyanoguanidine and b.) Melamine as well as degradation products generated by degradation of the formulation. Successful separation was achieved on a Phenyl Column using a mobile phase consisting of HPLC grade water to which 20µL of 10% TEA and: Solvent-X (90:10 v/v),were added. The flow rate was 1mL/min and detection was at wavelength of 232 nm. The methods have been validated with respect to linearity, accuracy, precision, specificity and robustness.

PP-449
COMPARATIVE DISSOLUTION STUDIES OF AN EXTENDED RELEASE FORMULATION OF TOLTERODINE TARTRATE AND TAMSULOSIN HCl

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ABSTRACT
A comparative study was undertaken on dissolution studies of marketed formulations which contain Tamsulosin HCl (TAM) and Tolterodine Tartrate (TOL) in a combination of 0.4 mg and 4.0 mg respectively in an extended release form. The dissolution method developed was then used to study three marketed formulations, quantification being done using a validated HPLC method. Comparison of dissolution data was done using the Moor and Flanner model independent method which included determination of Similarity factor and Difference factor. The kinetics of the dissolution process were determined by analyzing the dissolution data using four kinetic equations; namely Zero order, First order, Higuchi square root and Hixson Cube root equation. The results obtained were within the acceptance criteria. The kinetic study indicated that the dissolution data followed First order kinetics and Hixson Crowell cube root equation as straight line were obtained with a slope of approximately one and small value of intercept.

PP-450
A NOVEL APPROACH FOR GALLIC ACID PRODUCTION FROM *Terminalia* chebula BY ARISHTA METHOD

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ABSTRACT
Gallic acid (3,4,5-trihydroxybenzoic acid) is an organic substance occurring in many plants.It possesses wide range of biological activities, such as antioxidant, antibacterial and it is an important precursor for trimethoxybenzaldehyde which is used for the production of trimethoprim, a broad spectrum antibiotic.
Conventionally gallic acid is produced by acid hydrolysis of tannic acid but it has cost, yield and low purity. Alternatively, gallic acid can be produced by the microbial hydrolysis of tannic acid by tannase secreted by microorganisms.
Myrobalan is a main source for gallic acid.Thus has been used as a substrate for fermentation.

Aim of the present study is to propose a new approach to microbial Gallic acid production from Hirada arishta.Arishtas are alcoholic medicaments prepared by allowing their decoctions to undergo fermentation. Fermentation takes place by the addition of a source of sugar with *dhataki* (***Woodfordia fruticosa***) flowers on which the ***Aspergillus species*** resides.This microorganism releases tannase enzyme which is used for hydrolysis of tannic acid to yield gallic acid.The Gallic acid from the arishta was isolated with the help of organic solvents. The isolated compound after column chromatography gave a bluish green color with ferric chloride suggesting the compound to be a phenolic compound. The melting point and IR is similar to the reported in literature for Gallic acid. This confirms that the isolated phenolic compound is Gallic acid.

PP-451

EXTRACTION & SPECTROPHOTOMETRIC DETERMINATION OF PALLADIUM WITH CYANEX302

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ABSTRACT

A novel method is developed for the extraction and Spectrophotometric determination of Palladium using Cyanex 302 as extractant. Cyanex 302 is bis (2, 4, 4-trimethyl pentyl) monothiophosphinic acid. A method is developed for the extraction of Pd (II) in hydrochloric acid with Cyanex 302 in chloroform as an extractant. The optimum extraction conditions have been evaluated by studying parameters like HCl concentration, cyanex concentration, effect of diluents and period of equilibration. 0.7M Concentration of HCl and 0.08 M of cyanex 302 was found to give the quantitative extraction of Palladium. A study of equilibrium period on extraction established that extraction was quantitative after 45 seconds of equilibration. The Palladium-Cyanex complex showed maximum absorbance at 285 nm and no other chromomeric reagent was required. Beer-Lambert's law is obeyed in the concentration range of 30 to 180 µg with Sandell's sensitivity of 5.284x 10^{-3} µg/mL/$cm^2$and molar absorptivity 37,206 $mole^{-1}.cm^{-1}.dm^3$. A study of effect of diverse ions on the extraction showed that Sr(II),Mo(VI),Mn(II),Fe(III),Fe(II), Mg(II),Ce(IV),Sb(III) metal ions do not interfere during the extraction . Hence the selective extraction of Palladium from its binary mixtures containing mentioned above metal ions were done .The method is precise which can be seen from the RSD value of 0.28% for six replicate analysis which gave a mean absorbance of 0.755 for 100 µg of Palladium. The proposed method is simple, rapid, sensitive, precise and selective.

PP-452

KINETICS OF ß-GLUCURONIDASE USED FOR EZETIMIBE PHENOXY GLUCURONIDE HYDROLYSIS BY HPLC

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ABSTRACT

Enzyme kinetics is concerned with the measurement and mathematical description of the reaction rate and its association constants. Studying an enzyme's kinetics can reveal the catalytic mechanism of the enzyme and might prove helpful in controlling the activity of enzyme. Hydrolysis with ß-glucuronidase of the conjugated glucuronide, Ezetimibe Phenoxy Glucuronide (EZMG), liberated Ezetimibe (EZM). EZM was separated from possible interfering components in plasma through the use of HPLC and subsequently monitored with UV detection at 233 nm. The separation was performed on Kromasil C18 column (250 × 4.6 mm, 5µm) and the mobile Phase consisted of Acetonitrile and 1mM Ammonium Acetate in the proportion 60:40. The injection volume was 20 µL and the mobile phase was pumped at a flow rate of 1ml/min. The EZM production was monitored to assess ß-glucuronidase activity. The optimum temperature and pH for the enzyme-substrate reaction was optimized. Enzyme substrate saturation kinetics was studied in plasma upto 71.52 µg/mL of EZMG in plasma. A linear relationship of initial enzyme reaction velocity as a function of peak area of enzyme product was obtained for enzyme activity ranging from 10 to 500 units. Often a plot of the reaction velocity versus the substrate concentration is a hyperbolic curve as described by Michaelis-Menten relationship. However, ß-glucuronidase exhibited non-hyperbolic curve. We presume that enzyme is composed of subunits and exhibit cooperative kinetics and that the allosterism plays an important role in the regulation of enzyme activity.

PP-453

Expression of leukocyte adhesion molecules and phagocytosis in response to Nisin and Vitamin E plus Selenium treatment during acute bovine mastitis

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ABSTRACT

Phagocytic activity (PA) of milk polymorphonuclear cells (PMNs), concentration of interleukin 8 (IL 8) and expression of L selectin and CD 18 on peripheral leukocyte were studied in response to Nisin and Vitamin E plus Selenium treatment in cows inflicted with acute mastitis. The PA activity of the milk PMNs increased and concentration of IL 8 decreased in post treated cows (P<0.05). The expression of L selectin on peripheral PMNs was lower and CD 18 was higher in mastitic cows compared to healthy cows both before and after treatment (P<0.05).Whilst, the mean fluorescent intensity (MFI) of L selectin enhanced significantly in treated cows on day 7 (P<0.05), but CD 18 remained unchanged .The concentration of Selenium and Vitamin E was lower in mastitic cows. Serum Selenium concentration increased significantly in treated cows as compared to pretreatment values (P<0.05).

The results indicate that Nisin and Vitamin E plus Selenium therapy increases the PA and enhances the expression of L selectin and does not interfere with the expression of CD 18, both the parameters are related to enhancement of the mammary defense. Non antibiotic treatment along with Selenium and Vitamin E was effective in reduction of SCC and IL 8 from the inflamed udder compared to standard antibiotic treatment. Hence combination therapy of Nisin and Selenium plus Vitamin E may be recommended for the treatment of mastitis in such farming system where the antibiotics are not allowed. Furthermore development of such combination therapy is important in reducing the antibiotic residue from human food chain.

PP-454

MASKED-AMINO ACID: A NEW CARBON NUCLEOPHILE FOR RING OPENING OF ACTIVATED AZIRIDINES

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ABSTRACT

Aziridines have been synthetic targets as well as building blocks in organic synthesis since Gabriel's 1888 discovery of the smallest nitrogen-containing heterocycles.[1] In terms of synthetic transformations, the utility of aziridines derives from their selective ring-opening reactions, which often form the basis for more complex target syntheses.[2] Multifunctionalized ?-lactams are present as sub-structural units in biologically active substances and are also important intermediates for the synthesis of a variety of nitrogenated heterocycles that are considered as privileged scaffolds for drug discovery. Due to their versatile applications in organic and medicinal chemistry, the development of new synthetic routes for the preparation of pyrrolidin-2-ones is an important endeavor. Inspired by these valid points and keeping the synthetic and pharmacological importance of amide group in mind we turned our attention to utilize masked amino acid as substrates viz. 2-phenyl-1,3-oxazolan-5-one, which can introduce an amide group at a position into ?-lactam, which is the target molecule in the present investigation. we report a new molecular iodine catalysed one-pot atom efficient method for the preparation of 3-(N-substituted)aminopyrrolidin-2-ones **3** in a single step using [bmim]OH as a green reaction promoter. This one-pot synthetic protocol is highly atom efficient as there is no by-product formation and involves novel utilization of masked amino acid, 2-phenyl-1,3-oxazolan-5-one **1** with terminal aziridines **2** affording 3-(N-substituted) aminopyrrolidin-2-ones **3** in high yield and excellent diastereoselectivity in favor *cis* isomer (Scheme 1). Furthermore, the present synthesis of 3-(N-substituted)amino functionalized ?-lactam **3** is an outcome of our quest for developing new synthetic routes employing green chemistry protocols.[3] The formation of 3-(N-substituted) aminopyrrolidin-2-ones **3** can be rationalized by nucleophilic attack of the methylene carbon (C-4) of masked amino acid **1** to the less substituted carbon of tosyl aziridine **2** regioselectively, followed by protonation of aziridine nitrogen leading to the intermediate**.**

In conclusion, we have documented an original and practical regio- and diastereoselective route to synthetically and pharmaceutically important 3-(N-substituted)aminopyrrolidin-2-ones via nucleophilic aziridine ring opening with novel substrate viz. 2-phenyl-1,3-oxazolan-5-one. The efficacy of the reaction lies in its high yield, no by-product formation, ambient temperature, and recyclability of the ionic liquid [Bmim]OH. Thus, this simple methodology would be a practical alternative to the existing procedures for the production of this kind of fine chemicals to cater to the need of academia as well as of the industries.

PP-455

Nutraceuticals: Introduction, Importance and Review

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ABSTRACT

Nutraceuticals have received considerable interest in last two decade because of their presumed safety and potential nutritional and therapeutic effects. The term ***'nutraceutical'*** combines the word 'nutrient' (a nourishing food or food component) with 'pharmaceutical' (a medical drug) and coined by Dr. Stephen De Felice in 1989 to provide medical or health benefits including the prevention and treatment of diseases. The word 'nutraceutical' has been used to describe a broad list of products sold under the premise of being dietary supplements (i.e. a food), but for the expressed intent of treatment or prevention of disease. This term is being commonly used in marketing but has no regulatory definition. An attempt has been made to clear the concept of nutraceuticals and functional foods in this paper. The proposed definitions can help distinguish between functional foods, nutraceuticals, and dietary supplements. Nutraceutical scenario in India is also discussed in this paper.

PP-456

Rapid Stability Indicating UPLC method for Quantitative Analysis of Dronedarone Hydrochloride in Tables Dosage Form

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ABSTRACT

A simple, rapid, accurate, precise, sensitive and specific UPLC method is developed for the determination of Dronedarone in tablet dosage form. A new isocratic UPLC method is applicable for assay determination of the active pharmaceutical ingradient.The chromatographic separation is achieved within a short runtime of 3 minute using Acquity BEH C18 (100 mm *2.1 mm)1.7µm Column and 20mM KH_2PO_4 + 1mL Tri Ethyl Amine (pH=2.5 by Ortho phosphoric acid): Methanol (40:60) as a mobile phase at a 0.4 mL/min flow rate at 30ºC temperature.Peak detection is achieved with photodiode array detection at 290nm wavelength. The method was linear over the concentration range 20-80 µg/ml (r2 = 0.999) with a limit of detection and quantitation of 0.3 and 1.2 µg/ml respectively. Intraday and interday system and method precision were determined and accuracy was between 99.0- 101. %. The method was found to be robust and suitable for quantitative analysis of dronedarone hydrochloride in a tablet formulation. In Stability study of dronedarone, degradation products resulting from the stress studies did not interfere with the detection of dronedarone hydrochloride thus this method is stability indicating. Comparison of this method with HPLC method is made with respect to analysis time, efficiency and sensitivity.

PP-457

Synthesis of novel pyrido pyrimidine -2-ones derivatives

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ABSTRACT

Pyrimidine derivatives have found application in a wide range of medicinal chemistry because of their diverse biological activities, such as antimicrobial, antitumor and antifungal activities also these compounds are considered to be important for drugs and agricultural chemicals

In recent years, dihydropyrimidine-2(1*H*)one derivatives have gained much interest for their biological and pharmaceuticals Properties such as HIV gp-120-CD4 inhibitors, calcium channel blockers, a-adrenergic and neuropeptide Y antagonists, as well as antihypertensive, antitumor, antibacterial, anti-inflammatory agent. synthesize fused Pyrido[4,3-d] pyrimidine-2-ones having methyl sulfonyl group.

PP-458

One pot synthesis of benzylamine coumarin derivatives using PEG as a solvent and catalyst

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ABSTRACT

A green efficient and facile protocol was developed for the synthesis of a series of benzylamine coumarin derivatives by the reaction of 4-hydroxy coumarin, secondary amine and aromatic aldehyde in the presence of PEG as a solvent as well as catalyst at room temperature.A widw range of functional groups were tolerated in the developed protocol. The target molecules were obtained in good to excellent yield applying this method.

PP-459

Studies of different types of reactions on Pyrozole core structure

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ABSTRACT

2-Indolinone derivatives have recently been established as an anti-cancer compounds and more specifically as tyrosine kinase inhibitors (SU5416, SU5614, SU6668, SU6597, SU6663 and SU6561) that block kit activation and growth of small cell in lung cancer. Moreover Virsodia *et al* from our lab have reported the anticancer evaluation results of the arylidine products of 1-(2, 6-dichlorophenyl)-2-indolinone. Biological importance of such scaffolds inspired us to prepare new indolinone derivatives and to carry out their anticancer evaluation. 4-hydro xycoumarin is a versatile scaffold and is being consistently used as a building block in organic chemistry as well as in heterocyclic chemistry for the synthesis of different compounds. The synthetic versatility of 4-hydroxycoumarin has led to the extensive use of this compound in organic synthesis. 4-hydroxy coumarin shows diversified chemical reactivity and biological profile. Thus it was of interest to study the biological activities of newly synthesized coumarin derivatives.

PP-460

SYNTHESIS OF C-MANNICH BASES OF ARYLAMINOCOUMARINS: A NEW, NOVEL AND UNEXPLORED DIRECTION

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ABSTRACT

A new series of C-Mannich bases of 4-arylaminocoumarins was synthesized under affordable conditions. The Mannich reaction was carried out on 4-arylaminocoumarin derivatives at room temperature to obtain C-Mannich bases of 4-arylaminocoumarin derivatives. The Mannich reaction was fast and was easy to handle as well as to workup. The synthesized C-Mannich bases are new and prepared for the first time. The synthesized compounds were characterized by 1H & 13C NMR, FT-IR, Mass and elemental analysis.

PP-461
Stability Indicating RP-UPLC Assay Method and Validation of Amisulpride with Content Uniformity Study

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ABSTRACT
A reliable and sensitive isocratic stability indicating RP-UPLC method has been developed and validated for quantitative analysis and content uniformity study of Amisulpride in tablets. An isocratic method for analysis of Amisulpride was achieved on C18 (100 x 2.1 mm i.d., 1.7 µm particle size) column with flow rate 0.20 ml/min within shorter runtime 3 mins. Photodiode array detector was used to monitor the eluent at 280 nm. The mobile phase consisted of Buffer-ACN (50:50 v/v), (Buffer: 0.2% ortho phosphoric acid) is utilised to achieve good resolution and retention. The drug was subjected to oxidation, Alkali, hydrolysis, photolysis and thermal degradation. The detector linearity was established by concentrations range between 20-80 µg/ml (r^2=0.999) with a limit of detection and quantification of 0.1 and 0.3 µg/ml respectively. Recovery of drug was achieved between 99 to 101%. Degradation products resulting from the stress studies did not interfere with the detection of Amisulpride.

PP-462
CONVENTIONAL AND MICROWAVE ASSISTED SYNTHESIS OF NOVEL CYANO PYRIDINES

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ABSTRACT
Among a wide variety of heterocycles that have been explored for developing pharmaceutically important molecules such as cyanopyridines have played an important role in medicinal chemistry. They are reported to possess a broad spectrum of biological activity such as potential cardiovascular agents antiviral, CNS depressant18, bactericidal, ulcer inhibitors etc. Furthermore researchers have also revealed that cyanopyridine derivatives constitute an important class of compounds possessing diverse type of biological properties including antiviral, antiparasitic, antiparkinsonian, anticonvulsant, antihistaminic as well as anthelmintic properties.
The analogues of cyanopyridines were prepared by using 4-Hydroxy coumarine and pyrazole aldehydes with the application of conventional and microwave synthesis process. All the synthesized compounds have been confirmed by spectroscopic methods such as ^{1}HNMR, IR and Mass spectrometry. Further it is confirmed by elemental analysis.

PP-463
A MODULAR MULTI-DIVERSE APPROACH TOWARDS LIBRARY SYNTHESIS OF BENZODIAZEPINE MIMICS ON SOLID PHASE

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ABSTRACT
Benzodiazepines are potential bioactive agents due to their wide spectrum of therapeutic importance. A large number of substituted benzodiazepine derivatives are prepared and tested for varieties of biological activities such as anxiolytic, sedative, anticonvulsant, antithrombotics,etc.Benzodiazepines are an important group of bioavailable therapeutic agents with widespread biological activities. Due to their widespread biological activities and favorable pharmacokinetical properties, benzodiazepines were among the first classes of small molecules to be synthesized on solid support. The modular approach protocol has been developed for combinatorial solid-phase synthesis of benzodiazepine mimics. The merits of this solidphase protocol is less purification and free from tedious work up procedure. This minimize the time and accelerates the library synthesis. There is a scope of vast substrate availability and other point of diversity. All the synthesized compounds have been confirmed by spectroscopic methods such as ^{1}HNMR, IR and Mass spectrometry. Further it is confirmed by elemental analysis.

PP-464

One pot synthesis of Derivative of 2-phenyl trimethoxy Quinoline 4-carboxylicacid without catalyst

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ABSTRACT

A highly efficient and recyclable solvent method by Doebner reaction of 3,4,5-Trimethoxy aniline, pyruvicacid with substituted benzaldehyde is describe quinoline-4-carboxylicacid(1). Quinoline is heterocyclic fused ring containing benzene with pyridine is known as benzo[b] pyridine. Quinoline and their derivatives are possessed wide pharmaceutical and good biological activity. Quinoline 4-carboxylicacid is derivative of Quinoline. Quinoline 4-carboxylicacid and their analogous are a large number of natural products, drugs and prodrugs i.e. (angiotensin II receptor antagonist, neurokinin receptors). In Quinoline at 4-position carboxylic acid group directly introduced by Doebner reaction and Pfitzinger reaction. This methodology leads to synthesis 2-substituted Quinoline-4-carboxylicacid high yield (70-95%).Total 17 novel compounds were prepared.

PP-465

AN ISOCRATIC METHOD FOR QUANTIFICATION OF VALPROIC ACID AND ITS RELATED IMPURITIES USING ION PAIR REAGENT BY ULTRA PERFORMANCE LIQUID CHROMATOGRAPHY

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ABSTRACT

A selective Ultra Performance Liquid Chromatographic (UPLC) method for the quantification of Valproic Acid and its known related impurities using ion pair reagent has been developed. The method includes reversed-phase Acqutiy HSS T3 column with 100mm × 2.1 mm i.d. and 1.7µ particle size. The mobile phase consists of acetonitrile and 5mM 1-hexane sulphonic acid sodium salt in the ratio of (50: 50 v/v), flow rate is 0.6 ml/min and UV detection was performed at 215 nm. A System Suitability Test (SST) was developed to govern the quality of the separation. The developed method has been validated further with respect to linearity, accuracy, precision, selectivity, LOD, LOQ and robustness. The results were found satisfactory and within the limits.

PP-466

Use of Low Organic Contant Clay As Catalyst for the Organic Synthesis

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ABSTRACT

This paper reports of the use of low organic content clay as a catalyst for the synthesis of various organic reactions. Catalyst prepared by thermally activation and acidic treatment. Thermal activation is done at various tempreture where as acidic treatment is carried out by various inorganic mineral acid (HCl, H_2SO_4, $HClO_4$, H_3PO_4). Various morphological changes in clay properties achieved by thermal and chemically treatment of montmorilonite clay. Calcinations results increase in silica percentage of catalyst, crystalline structure, specific surface area and roughness of absorbant and catalyst recognisation is accomplished by various analytical techniques such as -XRD, FT-IR, SEM, and XRF. After acidic treatment bronsted acidity of clay is enhanced by Al-OH-Al and Si-OH-Al bondings. thermally and chemical treatment generates lots of activation on clay surface comparatively to untreated clay and it is use as heterogenous catalyst for the use of various esterification reactions. Product isolation and identification is carried out by GC-FID.

PP-467

Synthesis and Antibacterial activity of N-Mannich bases of 2-methyl indoline

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ABSTRACT

A simple, easy and fast method was adopted first time to prepare new N-Mannich bases of 2-methyl indoline using formaldehyde solution and primary and secondary amine. DEPT-135 experiment has proved the possible mechanistic path governing this reaction, which is probably hitherto unknown in literature. The newly synthesized compounds were screened for their antibacterial activity.

PP-468

Facile Synthesis of Some Novel Furo Coumarins

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ABSTRACT

Furo coumarins, such as Psoralene and the Angelicine derivatives are naturally occurring compounds produced by a variety of Plants, consist of a furan ring fused with coumarin. The main significance of the present work is that the molecules are synthesized in a pot synthetic process with reaction time ranging from 10 hr to 18 hrs. total fifteen derivatives of 2-(substituted 2-hydroxy benzoyl) 2,3-dihydro furo [3,2-c] chromen-4-one and 2-(2-hydroxy benzoyl) 3-(substituted phenyl) 2,3-dihydrofuro [3,2-c] chromen-4-one were synthesized. All the newly synthesized compounds are characterized by IR, NMR, Mass spectral data and elemental analysis. Furocoumarins are known to possess a high level of photobiological activity.

PP-469

Synthesis and Characterization of 5,6,7,8 substituted (3-Amido Adamantane) 4-Hydroxy Coumarins

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ABSTRACT

Browsing through the literature of medicinal chemistry the most useful moiety found was substituted 3-amino 4-hydroxy coumarin derivatives. Because of less toxicological properties and good to moderate activities, several compounds have been synthesized previously by our team. Though the chemistry of the synthesized compounds is known, the compounds are reported herein for the first time.

In the current work, two pharmacophoric moieties, coumarin and adamantane were converted into a hybridized structure by means of amide linkage. A new class of coumarin derivatives is generated and their potential biological activity will be checked upon. The synthesized compounds were well characterized by Mass, IR, and NMR spectroscopy.

PP-470
Synthesis & Biological evaluation of Imidazole derivatives bearing Quinoline nucleus

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ABSTRACT
Literature survey reveals that aryl amide derivatives have significant anti-tubercular activity in the field of pharmaceutical chemistry. These compounds are widely used as anticonvulsant, antianxiety, analgesic, sedative, anti-depressive, hypnotic agents and anti-inflammatory agents. In the last decade, the area of biological interest of amide linkage has been extended to several diseases such as cancer, viral infection and cardiovascular disorders. The above importance of pyrimidine leads us to synthesis arylamide derivative comprised with quinoline nucleus.
The present paper deals with the synthesis of aryl amide derive from hydrazide of quinoline and evaluation for antimicrobial, antitubercular and antifungal activity. The hydrazide have been prepared by the condensation of hydrazine hydrate with quinoline aldehyde which on condensation with different acid chloride to furnished aryl amide derivatives.
All the synthesized products have been confirmed by spectroscopic method such as ^{1}HNMR, IR and Mass spectrometry. It is further supported by elemental analysis. The synthesized products have been evaluated for antimicrobial as well as antifungal activity.

PP-471
Water Mediated Construction of Trisubstituted Pyrazoles/Isoxazoles Library Using Ketene Dithioacetals

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ABSTRACT
A small molecule library of alkyl, sulfone, and carboxamide functionalized pyrazoles and isoxazoles has been developed via a rapid sequential condensation of various R-acylketene dithioacetals (**1a-o**) with hydrazine hydrate or hydroxylamine hydrochloride, followed by oxidation of sulfide to sulfone using water as the reaction medium. An efficient and safe oxidation of sulfides (**4/5a-o**) to the corresponding sulfones (**6/7a-o**) using sodium per borate system in aqueous medium is reported. The concise and two step synthesis of trisubstituted pyrazoles and isoxazoles was investigated under variety of reaction condition. The newly developed methodology has the advantage of excellent yield and chemical purity with short reaction time using water as a solvent.

PP-472
1,3,5-Trisubstituted pyrazoline and 1,3,4-Aryl triazole derivatives of pyrazine 2-carboxylic acid: Synthesis and preliminary evaluation of biological properties.

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ABSTRACT
Pyrazine nucleus possesses remarkable pharmaceutical importance and biological activities. Pyrazine play an important role as intermediates for pharmaceuticals and chemical species. Extensive literature survey revealed very few published data on pyrazine derivatives as potential anti-inflammatory agents. This observation prompted us to synthesize this nucleus. Pyrazoline derivatives have attracted increasing attention due to their pharmaceutical applications such as antimicrobial [1], anticancer[2] and anti-inflammatory [3]. Aryl triazoles comprise a significant group of various heterocyclic compounds possessing promising biological activity in the area of medicine, which are known as potential anti- microbial [4], antidepressant [5], anti tubercular [6] agents. The importance of this study is to prepare various pyrazine2-carbxylic derivatives by introducing the pyrazine core into several molecules to explore the possibilities of some altered biological activities. A new generation of pyrazine hybrids bearing heterocyclic five membered ring such as 1,3,5- trisubstituted pyrazolines **(a)** and 1,2,4-Aryl triazoles **(b)** were designed and synthesized. The constitution of all the synthesized compounds have been characterized by FT-IR, ^{1}H NMR spectroscopy and further supported by mass spectroscopy. The purity of the compounds has been checked by thin layer chromatography.

PP-473

Synthesis and Anti microbial activity of thiopyrimidinederivatives bearingsubstituted quinolone derivatives nucleus

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ABSTRACT

During last decade, there is a considerable evidences have been observed to find potential of thienopyrimidines. To find the pharmaceutical importance of such a class of compounds as antibacterial agent[1] as well as antifungal agent [2-3], a series of thienopyrimidines derivatives have been prepared by condensation ketone and aldehyde with thiourea in the presence of alcoholic KOH as a catalyst. The present study deals with quinolones particularly 8-substituted which are associated with a post-antibiotic effect in a number of bacteria, principally gram-negative. All the synthesizedcompounds have been confirmed by spectroscopic techniques such as PMR, CMRand IR. Further supported by mass spectra and elemental analysis.The entiresynthesizedcompounds have been also evaluatedfor anti bacterial and anti fungal activity.

PP-474

Synthesis of some new imine derivative of 2-Thiobenzyl-1,3,4-thiadiazole and Preliminary Evaluation of Antimicrobial Activity

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ABSTRACT

Increasing treatment of multidrug resistant reached on alarming level in all over the world. So for the solution of this situation there is a need to develop anti infectious compounds.1,3,4-Thiadiazole ring containing compounds represent an important class of nitrogen containing heterocycles which possess broad spectrum of biological activity.

Thiadiazole ring is associated with many biological activities like anticonvulsant[1], antimicrobial[2], antitubercular[3], anti-inflammatory[4], cabonic anhydrase inhibitor [5] etc. 1,3,4-Thiadiazole exhibit broad spectrum of biological activities possibly due to presence of toxophoric N-C-S moiety[6].

Keep in view of all biological importance of title compound it is worthwhile to study the microbial activity of the stated moiety. In this study, we have synthesized the various imines by the reaction of 2-thiol-5-amino-1,3,4-thiadiazole with various chalcones derived from the furfural. The mercapto substitution of thidiazole reacts with benzyl bromide to give thiobenzyl derivatives. The constitution of all the synthesized compounds have been characterized by using elemental analysis and spectroscopic methods like FT-IR, ^{1}H NMR , Mass spectroscopy. All synthesized compounds are preliminary evaluate for antimicrobial activity.

PP-475

Synthesis of Some newer Heterocyclic Compounds as an Antimicrobial Agents

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ABSTRACT

Heterocycles continuous to be a major contributing nucleus in many of natural products and various intermediate building blocks in organic synthesis and thus have received significant attention for their preparation over decades. Heterocycles and their derivatives having sulpher and nitrogen as a heteroatom or both heteroatoms together have attracted attention of chemists mainly because of their broad spectrum biological and pharmacological activities. Thiazolidinone exhibits prominent structure in the field of pharmaceutical chemistry , possibly due to the presence of toxophoric N-C-S moiety. It is class of heterocycles which are potent inhibitor of Human Immunodeficiency Virus type-1 replication, cardio protective actions and antibiotic activity. These valid observations lead us to synthesize thiazolidinone derivatives fused with pyrimidine ring. The target molecule was synthesized by the condensation of thienopyrimidines with chloro acetyl chloride.

All the synthesized compounds have been confirmed by spectroscopic techniques such as PMR and IR. Further supported by mass spectra and elemental analysis. The entire synthesized compounds have been also evaluated for anti bacterial and anti fungal activity.

PP-476
Synthesis, antitubercular evaluation and Recursive partitioning analysis of some Imidazo[1,2-a]pyridine derivatives

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ABSTRACT
Imidazopyrimidine represent important building blocks in both natural and synthetic bioactive compounds which have shown to possess diverse therapeutic activities[1,2].The nature and the position of substituent's on the pyridine moiety influence these activity[3].Keeping this in mind, we have contemplated on the synthesis of pyrazolo derivatives bearing a imidazo[1,2-a]pyridine moiety. A series of pyrazole clubbed imidazo[1,2-a]pyridine have been synthesized by using the cyclo-condensation reaction of chalcones with hydrazine hydrate and their ability to inhibit growth of Mycobacterium tuberculosis in vitro have been determined. The results show that compounds ss-12 exhibited excellent anti-tubercular activity with IC-90 6.67 μg/ml where as other compounds exhibited moderate to good anti-tubercular activity. A classification SAR model was developed using recursive partitioning (RP) approach to identify the structural characteristics structural characteristics that could be tuned to improve activity. The decision tree derived from the RP model could identify and interpret the descriptors that discriminate imidazo[1,2-a]pyridine analogues.

PP-477
Stability Indicating HPTLC method for the Estimation of Agomelatine and in Tablet Formulation

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ABSTRACT
A simple, selective, precise and stability-indicating high-performance thin layer chromatographic method for analysis of Agomelatine in the bulk drug and in a tablet formulation has been developed and validated. Aluminum foil TLC plates precoated with silica gel 60F 254 were used as stationary phase. Dichloro methane and methanol in the ratio of (9.5:0.5v/v) were used as mobile phase. A compact band (R_f 0.52±0.002) was obtained for Agomelatine. Densitometric analysis was performed in absorbance mode at 230 nm. Linear regression analysis revealed a good linear relationship (r^2=0.9987) between peak area and concentration in the range of 0.2-0.8 μg /spot. The precision (relative standard deviation: RSD) among a six sample preparation was 0.79% and 0.81%. The accuracy (recovery) was found 100.62%, 99.70% and 101.01% respectively. The method was validated for specificity, linearity, precision, recovery, and robustness. The limits of detection and quantitation were also determined. Agomelatine was subjected to acid and alkaline hydrolysis, oxidation, photochemical and thermal degradation and underwent degradation under all these conditions. Degradation products produced as a result of stress studies did not interfere with the detection of agomelatine Statistical analysis proved the method enables repeatable, selective, and accurate analysis of the drug. It can be used for identification and quantitative analysis of Agomelatine in the bulk drug and in tablet formulations.

PP-478
Study of pharmacological activecyanopyran derivatives bearing Chloroquinoline nucleus

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ABSTRACT
Pyran core structure possesses the interesting biological activities, including analgesic, antimicrobial, antiviral, anti-inflammatory and antitumor. More over quinoline derivatives have prominent structure in medicinal chemistry. So it have stimulated considerable work in recent years advantage to synthetic utility of the various derivatives and large class of naturally occurring and synthetic biologically active pyran compounds made up of Chloroquinoline moiety.
With a view of getting better therapeutic activity, it wascontemplated us to synthesize pyranderivatives bearing quinoline moiety. The pyran derivatives have been prepared by the cyclo-condensation of chalcone[1] with malononitrile in pyridine.
All the synthesized compounds have been screened for their *in vitro* biological assay likeanti-Bacterial[2]and anti fungal[3] activity which is compared with standard drugs. Synthesized compounds have been confirmed by spectroscopic techniques such as PMR, CMR and IR. Further supported by mass spectra and elemental analysis.

PP-479
RP-HPLC method development and validation of Azilsartan medoxomil in human plasma

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ABSTRACT
Simple and fast reverse phase high-performance liquid chromatography (RP-HPLC) method using solid phase extraction technique by using strata-x cartridge (phenomenax) was developed and validated for the determination of Azilsartan medoxomil in human plasma. Chromatographic separation of the analyte Azilsartan medoxomil was achieved within 7.5 min by a waters symmetry C_{18} (4.6×250 mm, 5µm) column. The mobile phase consisting of 20 mM ammonium acetate buffer (pH 4.5)/acetonitrile (55:45, v/v) was pumped isocratically at a flow rate of 1.0 mL/min. The detection was carried out at 254 nm. Calibration curve was linear (r^2 > 0.9996) in the range of 1.0 –9.0 µg/mL. The overall mean recovery of Azilsartan medoxomil was 99.31%. Neither endogenous nor tested exogenous compounds were found to interfere at retention time of the analyte. This new RP-HPLC method may apply to clinical pharmacokinetic-based studies involving this drug, such as bioavailability/bioequivalence studies.

PP-480
Construction of 3,4-Dihydro-1,2-diazete Ring through 4p Electron Cyclization of 4-Hydroxy-2-oxo-2H Chromene-3-carbaldehyde[(1E)-arylmethylene] Hydrazone

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ABSTRACT
A new, short and efficient synthes is of 4-hydroxy-3-(4-aryl-3,4-dihydro-1,2-diazet-3-yl)-2H-chromen-2-one is described in which the 3,4-dihydro-1,2-diazete ring is constructed from arylmethylene hydrazoneby 4p electron cyclization as per electrocyclic reaction.

PP-481
Synthesis Of Some Novel Trifluoromethylated Tetrahydropyrimidines Using Etidronic acid and Evaluation For Antimicrobial Activity

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ABSTRACT
A simple and convenient, etidronic acid catalyzed, one-pot cyclocondensation reaction of 1, 3-diketone, arylaldehydes and urea to furnish trifluoromethyl tetrahydropyrimidine derivatives with excellent yield is described. The catalytic application of etidronic acid was investigated under various reaction conditions. All the synthesized compounds were evaluated for antimicrobial activity. The results obtained demonstrated that 40% of the synthesized compounds exhibited significant antimicrobial activity against all the tested micro organisms.

PP-482
PLA/ZrO_2 Polymer Nanocomposite synthesis and it's applications as drug carrier

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ABSTRACT
Polymer Nano composites are very well being used as drug carrier now days Lv and Tang et.al. [1-2]. Biodegradable Poly (lactic acid) (PLA) as polymer was used as a carrier and some inorganic metal oxide nanoparticles as fillers-binders Dabin and Shih et.al. [3-4]. In the current presentation PLA/ZrO_2 Nano composite synthesis via solution mixing method and characterization by DLS, powder XRD, IR and DSC. ZrO_2 used for the formation of Nano composite was of 100 nm (avg.) confirmed by DLS (particle size analysis) and powder XRD data shows the formation of Nano composite and further confirmed by thermal analysis and IR spectra. PLA/ZrO2 Nano composite studied for drug absorption by UV spectroscopy. The proposed structure of PLA/ZrO2 Nano composite is shown below.

PP-483

Use of Low Organic Content Clay as a Catalyst for the Organic Synthesis

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ABSTRACT

This paper reports of the use of low organic content clay as a catalyst for the synthesis of various organic reactions. Catalyst prepared by thermally activation and acidic treatment. Thermal activation is done at various tempreture where as acidic treatment is carried out by various inorganic mineral acid (HCl, H_2SO_4, $HClO_4$, H_3PO_4). Various morphological changes in clay properties achieved by thermal and chemically treatment of montmorilonite clay. Calcinations results increase in silica percentage of catalyst, crystalline structure, specific surface area and roughness of absorbant and catalyst recognisation is accomplished by various analytical techniques such as -XRD, FT-IR, SEM, and XRF. After acid ic treatment bronsted acidity of clay is enhanced by Al-OH-Al and Si-OH-Al bondings. Thermally and chemical treatment generates lots of activation on clay surface comparatively to untreated clay and it is use as heterogenous catalyst for the use of various esterification reactions. Product isolation and identification is carried out by GC-FID .

PP-484

Design and synthesis of novel phenanthridine derivatives as anticancer agents

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ABSTRACT

Cancer is unregulated cell growth forming malignant tumors, and invades nearby parts of the body. In 2007, cancer caused about 13% of human deaths worldwide (7.9 million) according to global cancer statistics. Benzo[*c*] Phenanthridine is naturally occurring alkaloid, which has anticancer activity through PARP-1 inhibition Makhey *et al.,* [1]. Also certain quinoline derivatives which have piperazine at second position exhibit antiproliferative activity Chih-Hua *et al.,* [2]. Many of the research groups predicted and reported that amide group can be replaced with a triazole ring which mimic and behave in the same fashion. The triazole ring exhibit anticancer activity and serves two purposes: (a) it facilitates stronger cap group interactions with the amino acid side chains at the entrance of the HDAC active site; (b) it serves as an isostere to the pharmacokinetically and toxicologically disadvantageous groups such as amide and ketone Chen *et al.,* [3]. Based on this background study, we strategically designed the new chemical entities. We coupled phenanthridinyl piperazines with various methylene triazoles and wanted to explore the synergistic effect of these heterocycles towards anticancer activity. A series of 6-{4-[(1-substituted-1*H*-1,2,3-triazol-4-yl)methyl]piperazin-1-yl} phenanthridine derivatives were synthesized in an effort to prepare novel anticancer agents. Among the synthesized compounds PT-3 and PT-7 were found to be more active compared to the standard drug etoposide. The compounds were synthesized either by microwave irradiation or conventional methods and were characterized by spectral techniques (IR, ^{1}H-NMR, ^{13}C-NMR and LCMS).

PP-485

"Synthesis and *in vitro* Antimicrobial Evaluation of Novel Fluorine Containing 3-Benzofuran-2-yl-5-phenyl-4, 5-dihydro-1*H*-pyrazoles and 3-Benzofuran-2yl-5-phenyl-4, 5-dihydro isoxazoles"

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ABSTRACT

Fluorine has become an invaluable tool for medicinal chemists because of properties it confers on molecules that contain it and biological activity it can create as a result. The ever increasing array of commercially available fluorinated starting materials coupled with novel synthetic methodologies offers to the synthetic chemists opportunities to positively influence the directions and timelines in a drug discovery programme. The use of fluorine to increase biological half life by impeding oxidative metabolism and to increase bioabsorption by lipophilic effects is the examples of directed strategies of fluorine

substitution. On the other hand chemistry of benzofurans in a large number of natural products has attracted attention due to their biological activities and potential applications as pharmacological agents as it represent a very important heterocyclic pharmacophore.

Thus we have synthesized some novel fluorine containing heterocycles incorporating benzofuran with dihydropyrazoles & dihydroisoxazoles and evaluated for their *in vitro* antimicrobial and antifungal activities. 2-Acetylbenzofuran on treatment with fluorinated aldehydes afforded corresponding fluorine containing 1-benzofuran-2-yl-3-phenyl-prop-2-en-1-ones **(**chalcones **5a-g).** The cyclocondensation of chalcones **(5a-g)** with hydrazine hydrate under basic conditions resulted in formation of corresponding novel fluorine containing 3-benzofuran-2yl-5-phenyl-4,5-dihydro-1*H*-pyrazoles **(6a-g)**. Similar reaction with hydroxylamine hydrochloride yielded 3-benzofuran-2yl-5-phenyl-4,5-dihydro isoxazoles **(7a-g).** All the synthesized compounds have been characterized on the basis of analytical and spectral data and were screened for their antibacterial and antifungal activities. Some of the synthesized compounds showed good antimicrobial and antifungal activities. Significance, Synthetic strategy, experimental details and characterization of these newly developed interesting molecules will be presented in the symposium.

PP-486

Supercritical Fluid Extraction and Identification of Flavonoids from *Nyctanthes arbor-tristis Linn* Leaves

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ABSTRACT

Plants produce a vast array of secondary metabolites, some of which exhibit pharmacological activities. Since these active compounds are usually present in low concentrations in plants, therefore development of more effective and selective extraction method of these compounds is needed. This paper describes the method for extraction and identification of flavonoids from *Nyctanthes arbor-tristis* leaves using Supercritical fluid (SCF-CO_2) technology. *N. arbor-tristis* leaf extract, used extensively in Indian traditional medicine, contains various substances that are considered to have health-promoting properties. Extraction of flavonoids from leaves, using ethanol as a modifier for SCF-CO_2, was undertaken. Various parameters such as temperature, pressure, CO_2 flow rate and Modifier concentration (ethanol) were studied. A UV spectrophotometric method was used for determination of flavonoid content under variable parameters which enabled optimization of the extraction conditions. The optimum extraction was achieved condition occurred at temperature 40°C, pressure 24.51 MPa, CO_2 flow rate 2ml/min and modifier 8.25%. The extraction yield obtained under optimized SFE conditions was 69.85%. The crude extract obtained at optimized conditions was further separated by performing Thin Layer Chromatography (TLC). The final optimized solvent system for TLC was Ethyl acetate: Methanol: Formic acid: Water (50:2:3:6) and qualitatively identified by specific reagent. Further Prep-TLC of separated bands was carried out and individual bands were analysed using HPLC. Mobile phase optimized for HPLC analysis consist of Methanol: ACN: Water [34:10:56] at flow rate of 0.4ml/min and injection volume 20µl. Further optimized SFE extract is examined for it's in- vitro antioxidant activity using DPPH radical scavenging assay.

PP-487

Macrocyclic Based Ditopic Molecular Receptor: A Novel Technology for Removal of Toxic Ionic and Organic species

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ABSTRACT

Toxic cationic, anionic and organic species are ubiquitous in nature and their presence in small quantities is essential for living systems. However they pose a serious threat to the environment and human health if they are present in excess or scarcity to a permissible limit [1-5]. The removals of these toxic ions are still a great scientific challenge due to their undistinguishable odor and color. Due to the high cost, least selectivity or sensitivity of available technology for removal of toxic ions requires to develop a more sensitive as well as cost-effective technology. Such sensor technologies are sorely needed by the monitoring, ecological, and environmental engineering communities. In this context, designing of a cost-effective but high quality macrocyclic based ditopic molecular receptor technologies [6-8] are one of the best choice for the sensing and then removal of

two toxic cationic, anionic and organic species [9, 10] from environments and water bodies with higher selectivity through allosteric effects wherein binding of one ion markedly influences the binding of the other ion [11, 12]. Calix[n]arene scaffolds [13, 14] would offer a suitable molecular architecture for novel ditopic molecular receptors, as they provide unique possibilities of assembling arrays of appropriate and complementary binding sites at both hydrophobic upper and hydrophilic lower rim as well as conformational characteristics for simultaneous recognition and extraction of two toxic ionic and organic species. A series of multisite molecular receptors have been synthesized by incorporating various functionalities into calix[n]arene scaffold either at the upper or lower rim. The simultaneous recognition and extraction studies for these receptors for various hazardous metal ions like Hg^{2+}, As^{3+}, Cr^{3+}, Cs^{2+}, Cd^{2+}, Pb^{2+}, Co^{2+}, Zn^{2+}, Ni^{2+} Mo^{+2} etc. and anions like F^-, Cl^-, Br^-, I^-, ClO_4^-, NO_3^-, AcO^-, HSO_4^- etc. have been completed by using UV-Visible, fluorescence and NMR studies and other spectroscopic techniques.

PP-488

Effect of nitrate poisoning on some biochemical parameters in Tilapia mossambica.

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ABSTRACT

The present study was conducted to investigated the toxicity of lead nitrate on Total Protein, Glucose, Cholesterol, Phospholipids, Acid Phosphatase activity and Alkaline Phosphatase activity in liver. Tilapia mossambica was used as an experimental model in the activity. It is divided into three groups and treated for 7,14 and 21 days as follows: Group I serve as control, Group II (experimental Group I 250 mg/ lit.); Group III (experimental Group II 500 mg/ lit.). The Total Protein in liver tissues of the experimental animals of Group III increased on 7th ,14th and 21st day but the values of the Total Protein were found to be statistically decreased and the values of the Glycogen content in the fish liver (Group II) were found to decreased on 7th day while on the 14th day and 21st day value differed non –significantly from that of the control Group. In Group III Glycogen content was non-significant as compared with the control group of animals . The value of Total Cholesterol in Group II were found to be increased on 7th day and 14th day and decreased on 21st day while the cholesterol content (Group II) decreased on 7th day and non–significantly increase and decrease was also seen on 14th and 21st day. The value of Phospholipids decreased in Group II but in Group III it was decreased significantly on 7th day and differed non-significantly on 14th and 21st day in comparision of Group I. The value of the Acid Phosphatase (GroupII) in the liver fish increased significantly on 7th day and decrease in 14th and 21st day while in GroupIII increased significantly on 7th and 14h day. Thereafter , a decrease in the 21st day. The value of the Alkaline Phosphate activity in the liver of the fishes of the experimental Group II was showed non-significant changes initially on 7th day whereas it is increased on 14th day and the enzymatic activity decreased on 21st day. The values of the Alkaline Phosphate activity on 7th and 14th day was non-significantly decreased on 21st day.

PP-489

Plant regeneration from callus culture of *Phyllanthus amarus* Schum and Thonn and *Asparagus racemosus* wild.

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ABSTRACT

Phyllanthus amarus Schum and Thonn (Euphorbiaceae) and *Asparagus racemosus* wild. (Liliaceae), commonly known as "shatavari" are important medicinal plant of herbal heritage of India. An efficient protocol has been developed for rapid mass propagation of *P. amarus* by callus derived from leaf explants. Optimal callus was developed from on Murashige and Skoog (MS) basal medium supplemented with low concentration of 2,4-D (1.0mg/L) . Adventitious shoots were regenerated (85%) from the callus on MS medium supplemented with 3.5mg/L Kinetin. Individual elongated shoots were rooted on half-strength MS medium containing 0.1 mg/L IBA. Regenerated plantlets with well developed shoots and roots were successfully transferred to soil. The developed callus can also be used for large scale production of phyllanthin and hypophyllanthin. Similarly, embryogenic calli were induced from nodal segments of *A. racemosus* on half strength Murashige and Skoog medium supplemented with 2.0 mg/L 2,4-dichlorophenoxy-acetic acid (2,4-D) and 1 mg/L **TDZ**. Mature somatic embryos were converted to plantlets on MS medium supplemented with low concentration of BAP (0.5 mg/L). The developed protocol would be useful for mass propagation and large scale propagation of *P. amarus* and *A. racemosus.*

PP-490

SYNTHESIS, ELECTRICAL AND THERMAL PROPERTIESOF $Bi_4V_{2-x}Cu_xO_{11}$ (x=0.0 and 0.06) CERAMICS

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ABSTRACT

Polycrystalline ceramic samples of pure and Cu^{+2}doped $Bi_4V_{2-x}Cu_xO_{11}$(x=0.0 and 0.06) have been synthesized by standard solid state reaction method using high purity oxides.The dielectric constant and dielectric loss and hence ac conductivity as a function of frequency and temperature have been measured. The dielectric studies indicate that the material is highly lossy and hence its ac conductivity increases with the increase of temperature. The dc conductivity of material has been measured as a function of temperature from room temperature to 653K and its activation energy was calculated using the relation $s = s_o exp (-Ea/kT)$.The Modulated Differential Scanning Calorimetry (MDSC) has been used to investigate the effect of substitution on the phase transition of the compounds. The results are discussed in detail.

PP-491

BIOCHEMICAL STUDY OF ADAPTOGENIC PROPERTY OF *Withania somnifera* IN RAT BRAIN AFTER STRESS

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ABSTRACT

The biochemical effect of *W.somnifera* were studied on stressed and non stressed albino rats. Experimental rats were subjected to immobilization stress for 14 hrs and treated with herbal extracts. Animals were sacrified by decapitation and blood were collected for serum to estimate corticostreroid level, SGOT (serum glutamate oxaloacetate), SGPT (serum glutamate pyruvate transaminase),NBT reduction test. The brain was quickly removed from braincase and placed in ice cold phosphate buffer saline and used for study of AchE (Acetylcholine estrase), BchE (Butylcholine estrase), Ascorbic acid and total protein content. Results demonstrated that acute and chronic stress affects the corticosteroid, SGOT, SGPT level and the values can be brought back to normal by treatment of *W.somnifera. W.somnifera* is strong antioxidant and may be helpful in stress condition as an antistress.

PP-492

A novel synthesis of 4-amino-3-aroyl/acetyl-2-methylsulfanyl-napthalene-1-carbonitriles

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ABSTRACT

1-Amino-naphthalene-2-yl-phenyl-methanone derivatives exhibit broad spectrum of biological activities, such as antitumor, anticancer, and antiproliferative activity.[1] These aryl naphthyl ketones were synthesized by reaction of 2-amino-5-chlorobenzonitrile and Grignard's reagent, 1-naphthylmagnesium bromide, in diethyl ether.[2] Since very few literature procedure are available for synthesis of these compound which involves harsh reaction conditions. A novel synthesis of 4-amino-3-aroyl/acetyl-2-methylsulfanyl-napthalene-1-carbonitriles have been carried out by reaction of of 2-(1-cyno-2,2-bis methylsulfanyl vinyl)-benzonitrile[3] and various aryl methyl ketones under basic reaction conditions. Precursor can be synthesized by reaction of 2-cyanobenzylcyanide with carbon disulphide and methyl iodide under basic conditions at 0 ^{0}C. In an alternative approach desired mo lecule can be synthesized by reaction of 2-cyanobenzylcyanide with 3,3-bis(methylthio)-1-arylprop-2-en-1-one under similar reaction conditions.

PP-493

Synthesis and Characterization of L-Prolinamide Based Chiral Mn(III) Salalen Complexes and Their Applications in Asymmetric Catalysis

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ABSTRACT

Chiral Mn(III) Salen complexes are quite efficient catalysts for asymmetric epoxidation of non-functionalized olefins.[1] We have synthesized new Mn(III) Salalen complexes for the asymmetric epoxidation and other asymmetric transformations. We earlier used Mn(III) Salen complexes means analogues of Jacobsen Mn(III) Salen complexes for the asymmetric epoxidations.[2] These complexes were synthesized by the reaction of prolinamideSalalen ligands and $Mn(OAc)_2.3H_2O$ under inert atmosphere. These complexes were characterized by IR, CHN, Mass Spectroscopy and Cyclic voltammetry.

PP-494

SYNTHESIS, CHARACTERIZATION & BIOLOGICAL ACTIVITY OF Co(II) COMPLEXES OF HYDROXYTRIAZENE DERIVATIVES

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ABSTRACT

A series of hydroxytriazenes having identical composition based on chloro fluoro substituents has been synthesized via diazocoupling of diazonium salt with hydroxylamine[1]. Synthesized hydroxytriazenes was used for preparation of Co(II) complexes. The chemical composition was assigned using different spectroscopic methods. The complexation of hydroxytriazenes has been monitored using spectrophotometeric methods[2]. In acetonic solution 1:2 stoichiomemtery were established by molar ratio method and Job's continuous variation method. A tetrahedral geometery has been suggested for all the complexes. All the Hydroxytriazenes and their Co(II)-complexes were tested for antimicrobial activity against *Pseudomonas aeruginosa, Staphylococcus aureus* (Bacteria), *Candida albicans, Cryptococcus neoformans, Sporothrix schenckii, Trichophyton mentagrophytes, Aspergillus fumigatus and Candida parapsilosis* (ATCC-22019) (fungi). The MIC (Minimum inhibitory concentration) values vary from as low as 1.56µg/ml to 50µg/ml. Thus the present study has been planned on bioactive metal complexes[3,4].

PP-495

Nanomaterials for sensing of heavy metal ions in aqueous media

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ABSTRACT

SiO_2@Au and Au@citrate NPs have been synthesized by successive reduction of metal salts on pre-made core, reduction of metal salts by suitable reducing agent ($NaBH_4$) and reduction of metal salts by reductants in the presence of a cationic surfactant, cetyltrimethylammonium bromide (CTAB), respectively. The coverage of the seeds is extremely uniform, although in some cases deviations from a spherical shape are observed with the formation of nanorods or nanoprisms. In present work, we concentrate on developing the sensor materials for heavy metal ions detection which are fast, simple and usable by non-experts. We were also discussed the chemical interactions of toxic metal ions such as Cd(II), Zn(II), Fe(III) and Pb(II) with subjected nanomaterials and effect of metal ion concentration as well as pH of the medium on their interaction. We have studied the effect of interaction using spectroscopic and microscopic techniques such as UV-VIS, SEM, TEM and in detail by SERS. The crystal violet (CV) served as the SERS readout molecule and the modified tag to attach on the gold nanoparticles and gold nanoparticles were linked through the heavy metal ions (Cd^{2+}, Pb^{2+} and Fe^{3+}) thus sandwich structure was built for detection.

PP-496

Constituents of *Annona squamosa* twigs having major immune modifier to elicit polarized Th1 immune response in BALB/c mice

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ABSTRACT

Annona squamosa L. (Annonaceae) has traditionally been used as herbal medicine, commonly known as Custard apple, Sweetsop or Sugar apple is a native of Central America and is widely cultivated throughout India [1]. It has various traditional medicinal uses for the treatment of diabetes, epilepsy, cardiac problems, constipation and ulcers [2-5]. Till date there is no report on the compounds responsible for the immune-stimulatory activity of this plant. Present communication deals with the phytochemical analysis and pharmacological investigation of the most active chloroform fraction that led to isolation and identification of a number of compounds whose structures were elucidated using 1D and 2D NMR spectroscopic analysis. Amongst the twelve pure compounds isolated, five compounds Lanuginosine (1), (+) -O- methylarmepavine (2), (+)-anomuricine (3), Isocorydine (4), and N-methyl-6,7-dimethoxyisoquinolone (5) were evaluated *in vivo* for their immune modifier activities in BALB/c mice after oral administration at three log doses of 0.3, 1.0 and 3.0 mg/kg for 14 consecutive days. Of these, three compounds (1, 2 and 5) showed dose dependent immune stimulating activity. However, the highest activity was noted in the compound N-methyl-6, 7-dimethoxyisoquinolone at the 3.0 mg/kg oral dose. The compound possibly acted modifying the expression of Th1- and Th2- cytokines via stimulation of pro-inflammatory Th1 cytokines IL-2 and IFN-?. These results explore the use of the above compounds as an efficient immune-stimulant or immune-adjuvant against diseases with immune suppression.

PP-497

SYNTHESIS CHARACTERIZATION AND ANTIMICROBIAL ACTIVITY OF HYDROXYTRIAZENES

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ABSTRACT

The present work reports synthesis characterization and antimicrobial activity of hydroxytriazene derivatives. The hydroxytriazenes containing trifluoro moiety have been synthesized by diazocoupling reaction with phenylhydroxylamine[1]. The composition of all hydroxytriazene derivatives has been assigned by CHN and IR spectral analysis. All the hydroxytriazenes have been screened for antibactrerial and antifungal activity[2,3]. Thus the present work has been planned to synthesize biologically active hydroxytriazenes.

PP-498

Synthesis of hydromagnesite rectangular thin sheets & its application as novel catalyst in one-pot synthesis of 2-aminochromene derivatives *via* Knoevenagel condensation

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ABSTRACT

Rectangular hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$) thin films [1,2] was synthesized by a facile and environmentally friendly hydrothermal route from $Mg(NO_3)_2$ and characterized by by powder XRD, TG-DTA, FT-IR, SEM, EDAX, HR-TEM, BET analysis and photoluminescence (PL) studies. Hydromagnesite thin sheets was explored as heterogeneous base catalyst in one-pot synthesis of 2-aminochromenes [3-6] *via* Knoevenagel condensation. The excellent catalytic potential of hydromagnesite was due to unusual reactive thin plate morphology and high BET surface area($250 m^2/g$).

PP-499

SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL EVALUATION OF SOME *N*'-(4-(2-(2-PHENYLACETYL)HYDRAZINYL)- 6-(ARYLAMINO)-1,3,5-TRIAZIN-2-YL)ISONICOTINOHYDRAZIDES AND *N*'-(4-(2-(2,4-DICHLORO BENZOYL)HYDRAZINYL)- 6-(ARYLAMINO)-1,3,5-TRIAZIN-2-YL) ISONICOTINO HYDRAZIDES

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ABSTRACT

1, 3, 5-Triazine derivatives have been known for widespread applications in the pharmaceutical. Several s-triazine derivatives showed chemotherapeutic activity such antibacterial, fungicidal, antimicrobial, antimalarial, anticancer, antiviral, anticonvulsant etc. Isoniazid is also an important bioactive moiety and it is active against *Mycobacterium tuberculosis*. Looking to the pharmacological importance of s-triazine and isoniazid we tried to incorporate both pharmacophores in single frame for enhancing antimicrobial activity. We have synthesized series of *N'*-(4-(2-(2-phenylacetyl)hydrazinyl)-6-(arylamino)-1,3,5-triazin-2-yl) isonicotinohydrazides and *N*'-(4-(2-(2,4-dichlorobenzoyl)hydrazinyl)-6-(phenylamino)-1,3,5-triazin-2-yl)isonicotinohydrazides. All the synthesized compounds were screened for *in vitro* antibacterial and antifungal activities on *Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, Staphylococcus pyogenes, Candida albicans, Aspergillus niger* and *Aspergillus clavatus.* The structures of the compounds synthesized were elucidated by IR, ^{1}H-NMR,^{13}C-NMR and mass spectra.

PP-500

Synthesis, characterization and thermal study of 4-oxo-thiazolidine derivatives

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ABSTRACT

Three compounds of 4-oxo-thiazolidine derivative were synthesized by condensation reaction. These synthesized compounds ($AJ5_{c\text{-}e}$) have been characterized by various spectral techniques such as FT-IR, ^{1}H-NMR, ^{13}C-NMR and mass spectroscopy. The thermal stabilities of these compounds ($AJ5_{c\text{-}e}$) were investigated by simultaneous TGA and DSC methods. The decomposition steps and thermal behaviour of three compounds were investigated. The kinetic parameters such as order of reaction (n), energy of activation (E_a), pre-exponential factor (A), entropy of activation ($\Delta S^{\#}$), enthalpy of activation ($\Delta H^{\#}$) and Gibbs free energy of activation ($\Delta G^{\#}$) were evaluated by using Freeman-Carroll method. The one step degradation for each compound and its correlation with thermal behaviour were also evaluated.

PP-501

Pharmaceutical properties of natural hydrophilic gum polymers

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ABSTRACT

Guar Gum, initially was used only as disintegrant and binder in the tablet, now, is used as a controlled release agent for drugs. Drugs with natural polymers like guar gum in powder form are mixed with other ingredients and compressed to form tablets. Dissolution of the same results in the hydration of guar gum and formation of a thick layer of gel on the surface of the tablet. These natural gums are biodegradable and non-toxic[1,2].

In the present investigation, influence of particle size on viscosity of guar gum was determined, which plays a very significant role in controlling the release of drug. Maximum viscosity was obtained for 200 mesh particle size.It has been established that hydration kinetics is determined by particle size as it reflects the changes in surface area exposed to water.

PP-502

Eco-Friendly Natural Additives for Rubber Products

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ABSTRACT
Globalization of Indian market through liberal economic reforms has successfully created great influence on the overall development of our society. An unprecedented growth in consumer demand and corresponding industrial growth is inevitable. The trend is poised to be sustained for at least next few decades. Materialistic life style of all individuals is well reflected; compelling researchers and industrialists to search & develop newer material and products for progressive global market. So is the rubber industry. Thousands of rubber products are marketed for variety of applications. India is annually using more than 3 million MT of rubber. However looking to mass population and relatively lower mass capita consumption in comparison to developed countries, it is expected to increase many fold in next couple of years. In contrast to most of the other class of polymers production of rubber products is a complex process, utilizing many other ingredients to ease its processing and make the product for better application as well as for longer service life. All synthetic rubbers and rubber additives currently being used are based on petroleum. Depletion of petroleum stocks and emission of particulate and non-particulate materials from rubber products; during their production and their service life greatly threaten us to search for newer, eco-friendly and sustainable materials. This study is to report characterization of some of these additives extracted from plants and. Some of these processing aids and processing oils used shows comparable physical and mechanical properties with those of the conventionally used petroleum based additives.

PP-503

Study of Antidiabetic Properties of *Tinospora Cordifolia*

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ABSTRACT
Diabetes is observed when there is alteration in activities of different enzymes related to carbohydrate metabolism. Increased oxidative stress is observed in diabetes, it is observed when there is imbalance between free radical scavenging capacity of antioxidant defense mechanism. The pharmacological principles in *Tinospora cordifolia* the work in dynamic way to produce maximum therapeutic efficacy with minimum side effects. The present study was to evaluate antidiabetic property of extract of *Tinospora cordifolia* & its role in reducing enzyme activity altered in diabetic complications. Aqueous and ethanolic extracts of *Tinospora cordifolia* were subjected to phytochemical screening. The quantitative analysis of phenolics and flavonoids was carried out using spectrophotometry and High Performance Liquid Chromatography. Enzyme activity of a-amylase and a-glucosidase was also studied spectrophotometrically, The high amount of phenolics and flavonoids present in the *Tinospora cordifolia* extract suggest their antioxidant potential and reduced enzyme activity of a-amylase and a-glucosidase suggests presence of phytochemicals responsible for controlling glucose metabolism. Therefore *Tinospora cordifolia* extract could be an alternative mode in treatment of hyperglycemia.

PP-504

Use of Guar Gum in the drug delivery systems

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ABSTRACT
Natural gums are popular hydrophilic polymers, because, when in contact with aqueous medium they gradually hydrate from periphery towards the centre resulting in gelatinous swollen mass. The diffusion of drug molecules into the aqueous medium through the polymeric material is controlled by this mass (Colombo *et al.*). The objective was to study suitable properties of guar gum to develop sustained release tablets. The drug release mechanism from guar gum follows Fickian diffusion i.e. drug release is by water penetration, gelatinization and diffusion (Shaikh *et al.*). In the present investigation, influence of pH on viscosity of guar gum was determined, which plays a very significant role in controlling the release of drug.
Maximum viscosity was obtained for pH ranging from 6-7 (almost neutral) ,whereas, before and after this pH , a gradual decrease in viscosity was accounted. This could be attributed to partial hydrolysis of polysaccharides by acid/alkali resulting in decrease in the molecular weight.

PP-505

Synthesis of a Blue Phosphor ZnO@Ga_2O_3 by a combustion method and its application as at UV light excitation

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ABSTRACT

Undoped solid solution ZnO@ Ga2 were successfully synthesised in a pure monoclinic phase by combustion method , using urea as a reducing agent at 400°C temperature These solid solution were found to be exhibit a good blue emission (452 nm) under UV excitation (345nm)..defects generated were found to be responsible for photo luminisence character. Advance techniques of characterisation was used to investigate the compound i.e. .XRD CIE, DRS, FESEM.. TGA/DSC were used to explore the synthesis mechanism compound.

PP-506

A NEW SYNTHETIC APPROACH AND *IN VITRO* ANTIMICROBIAL EVALUATION OF IMIDAZOLINE INCORPORATED THIAZOLIDINE MOTIFS

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ABSTRACT

The emergence of microbial strains resistant to the present antibiotics highlights the need for search of new antimicrobial. In continuation to this, the present paper deals with the synthesis and antimicrobial activity of a novel series of **2-[1,2-diaza-3-(4-{4-[(aryl)methylene]-2-(4-nitrophenyl)-5-oxo(2-imidazolinyl)}phenyl)but-2-enylidene]-1,3-thiazolidin-4-ones**. The structures of these compounds were characterized by spectral (IR, ^{1}H-NMR, ^{13}C-NMR, mass spectra) analysis. All bio-active molecules were tested for their *in vitro* antimicrobial activity by bioassay namely serial broth dilution. Compounds were screened for *in vitro* antibacterial activity against the representative panel of Gram-positive (*Staphylococcus aureus*, *Streptococcus pyogenes*) and Gram-negative (*Escherichia coli*, *Pseudomonas aeruginosa*) bacteria. All newly synthesized compounds were also tested for their inhibitory action against three strains of fungi (*Candida albicans*, *Aspergillus niger*, *Aspergillus clavatus*) and have exhibited moderate to excellent growth inhibition of bacteria and fungi. On basis of statistical analysis, it was observed that these compounds showed significant co-relation.

PP-507

Design and Synthesis of Substituted Quinolones as Potential Cytotoxic Agents

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ABSTRACT

Cytotoxic agents are commonly used in chemotherapy to inhibit the proliferation of cancerous cells. 4-Hydroxy-2-quinolones are important class of compounds that exhibits a variety of interesting pharmacological activities such as antibacterial, antimicrobial, anti- HIV, antiviral and antitumor. Recently, these compounds have been described as selective NMDA antagonists with potent *in vivo* activity after oral administration. The present work explores the naturally occurring alkaloid, casimiron as a core scaffold to synthesize new class of cytotoxic agents based on pyranoquinolone scaffold. The targeted pyranoquinolones were synthesized by reaction 4hydroxy-*N*-methylquinolines with substituted benzylidenes under basic condition in DMF at 80°C. New series of compounds has been evaluated for cytotoxic activity using MTT assay on colon cancer cell lines (COLO-205). Compounds bearing nitrile group were found to be more potent than the compound bearing ester group.

PP-508

Interaction of an Amphiphilic drug Trifluoperazine Dihydrochloride (TFP) with Triblock Copolymers

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ABSTRACT

A most common challenge faced by pharmaceutical scientists as well as industry is to design and develop drugs with good aqueous solubility while simultaneously retaining potency and selectivity. The concentration of drug should be high enough at the targeted site to facilitate the therapeutic effect, but simultaneously it should not be too high, because this may result in unfavourable side effects[1]. Trifluoperazine dihydrochloride (TFP) also suffers from several drawbacks such as anticholinergic, cardiovascular and antiarrhythmic side effects. These undesirable side effects may be reduced if the drug is properly targeted to the organism [2]. In this context, Pluronic Triblock copolymers have appeared as substantial vehicles for controlled drug release in comparison to other alternatives . They can solubilise poorly soluble drugs in their hydrophobic core, thus increasing their bioavailability [3]. Also, these micelles protect drugs from destructive factors upon parenteral administration, modify their biodistribution and their (micelle) sizes permit them to accumulate in areas with leaky vasculature. Polymeric micelles are kinetically stable so they dissociate slowly, even at concentrations below the CMC, extending circulation times in blood. In addition they display larger cores than surfactant micelles, leading to higher solubilisation capacity than the regular micelles[4]. So, the present work was conducted in order to have an overview of effect of triblock copolymers such as L64, P123 and F68 on the physicochemical properties of antidepressant phenothiazine drug, trifluoperazine dihydrochloride. Surface tension measurements have been done in order to study the nature of interactions between drug-triblock copolymers. The various interfacial, micellar and corresponding thermodynamic parameters have been calculated. The value of thermodynamic parameter ($?G_t^o$) calculated from cloud point studies indicates that the phase separation process is spontaneous for mixtures of TFP and triblock copolymers.

PP-509

Estimation of Uranium Uptake And Bioaccumulation In Different Plant Samples In Bathinda And Suratgarh Thermal Power Station, India.

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ABSTRACT

The paper describes uranium uptake by different plant species The concentration of the Naturally Occurring Radioactive material (Norm) mainly uranium is analyzed in different plants namely-Ganda (Tagetes spp.), Jamun (Syzgium cumini), Gudhal (Hibiscus species), Rose (Rosa indica L.), Sudarshan (Crinum spp.), Sadabahar (Catharanthus Roseus), Kela (Musa spp.) and Guldawari. These were collected from Guru Nanak Dev Thermal Plant, Bathinda and Suratgarh Super Thermal Power Station, Suratgarh. Analysis of uranium concentration is done by ICP-MS (Inductively coupled plasma – mass spectrometry) in IIT-Roorkee with multielement standards. Eight different plants were collected (between July, 2010 to May, 2012) in the two thermal plants. Uranium concentration is in the range of 15.7 to 2165.3 ppb. Maximum uranium is found in the root of Tagetes spp. 2165.3 ppb or 2.16 ppm and minimum uranium was accumulated by root of Crinum spp.that is 15.7ppb. It is relevant to indicate that the uranium concentration is high in Tagetus plant and it can use for phytoremediation due to high capacity of accumulation of uranium. The result indicates an elevation of Norm content in both thermal plant due to Thermal plant establishment or any other reasons in that area.

PP-510

Diversity-Oriented Synthesis of Dibenzoazocines and Dibenzoazepines via a Microwave-Assisted Intramolecular A3-Coupling Reaction

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ABSTRACT

In light of the increased demand for the diversity-oriented [1] generation of biaryl-containing medium-sized rings, [2] different approaches have been developed to synthesize these biologically interesting classes of compounds. One of the example is Buflavine, comprises a biaryl-containing medium-sized rings and exhibits an interesting biological activities such as α-adrenolytic and antiserotonin activities.[3-5] Therefore, we have presented here an unprecedented, diversity-oriented strategy for the generation of 6,7-dihydro-5*H*-dibenzo[*c,e*]azepines and 5,6,7,8-tetrahydrodibenzo[*c,e*]azocines by a microwave-assisted copper-catalyzed intramolecular A3-coupling reaction.[6] Further, we investigated A3 couplings via the intramolecular reaction of biaryl compound **1** that was *in situ* formed via Boc deprotection. The latter intermediate delivers both the aldehyde and the amine moiety, which were reacted with acetylene **2** using CuBr as the catalyst in toluene under microwave irradiation to yield **3** (Scheme 1). This intramolecular A3-coupling process was also performed with copper-in-charcoal (Cu/C) under continuous flow conditions. Transferring the conditions from the microwave batch experiment to continuous flow process gave good yield of the desired intramolecular A3-coupling product.

PP-511

Microwave in the Total Synthesis of Natural Products

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ABSTRACT

Total synthesis of natural products is one of the difficult tasks for organic chemists because of their complex structures and difficult stereochemistry. Many scientists around the world have putting their best efforts and ideas to synthesize these complex structures with the help of new technology [1]. Natural product's synthesis by the conventional method is a long process which sometimes includes various side reactions and poor yield. Microwave irradiation is a powerful tool to reduce the reaction time and improve the product yield and purity as compared to the conventional heating methods. In this presentation, we have highlighted some of the exciting research article that has significantly improved the yield and reduced the overall synthetic time. One of such the example has shown in scheme-1.[2]

PP-512

Design, Synthesis and *in-vitro* Evaluation of Polymeric Prodrug of Gemcitabine for Colon Cancer

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ABSTRACT

Colon cancer is the third most common cause of cancer and second leading cause of cancer-related deaths in the western world [1]. There are number of effective anticancer drugs but these are neither site specific nor free from adverse toxic side effects [2]. Gemcitabine is an antimetabolite drug used in treatment of various types of cancers but it has some side effects like loss of appetite, thinned or brittle hair, constipation etc. With the increase thrust of Gemcitabine in cancer chemotherapy, novel polymeric prodrug of Gemcitabine **(4-[(4'-aminophenyl azo)-1-(3'', 3''-fluoro-4''-hydroxymethyl tetrahydrofuran-2''-yl)]-pyrimidine-2-one)** having site specificity to colon have been designed, synthesized and characterized by modern analytical techniques. Prodrug was designed having azo linkage because azo reductases present in the colonic microflora. These enzymes cleave the azo bond and release the targeted drug to colonic site. *In-vitro* release profile of polyphosphazene (polymer) linked prodrug of gemcitabine were studied at pH 1.2 and pH 6.8 to check the release behavior of drug in acidic pH and at basic pH. The result showed that polyphosphazene linked prodrug of gemcitabine has 90.85% release at pH at 6.8. Therefore, Polyphosphazene linked prodrug of Gemcitabine having azo linkage seems to be the most promising candidate and is selected for further drug designing having site specificity.

PP-513

Design, Synthesis and *in-vitro* Evaluation of Novel Analogues of Oxaliplatin for Colon Cancer

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ABSTRACT

Development of novel platinum(II) complexes is an important era in the treatment of cancer. Oxaliplatin is third generation platinum based anticancer agent which has *trans*-(±)-1, 2-diaminocyclohexane (DACH) [1, 2]. In spite of its success, it has several disadvantages such as nephrotoxicity, neurotoxicity, ototoxicity and the appearance of resistance in cancer cell lines [2]. With the increase thrust of platinum complexes in cancer chemotherapy, we have synthesized the novel platinum based anticancer compounds (**2-4**) having phthalate as the leaving group have been designed, synthesized and characterized by modern analytical techniques.Platinum(II) complexes (**2-4**) were evaluated *in-vitro* on COLO 205(human colon cancer cell line) against parent drug oxaliplatin, which showed that all the synthesized molecules (**2-4**) have better cytotoxicity property in comparison to oxaliplatin, but the **4-amino-(trans-cyclohexane-1,2-diamine)phthalate platinum(II) (4)** showed maximum activity **(IC_{50}=0.12**) and is more active than oxaliplatin **(IC_{50}=0.19**). Therefore, 4-amino-(trans-cyclohexane-1,2-diamine)phthalate platinum(II) (**4**) is the most promising candidate and is selected for further drug designing and *in-vivo* evaluation in future.

PP-514

PHARMACOLOGICAL PROFILES OF A NOVEL PROTEIN TYROSINE PHOSPHATASE 1B INHIBITOR

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ABSTRACT

Protein tyrosine phosphatase 1B (PTP-1B) act as a negative regulator of insulin signaling and selective inhibition improves the insulin sensitivity (Fukuda *et al*., 2010). Therefore PTP1B inhibitors represent attractive pharmaceutical agent for type 2 diabetes and obesity (Pandey *et al*., 2011). A series of novel PTP-1B inhibitors was discovered containing sulphonamide. Structure–activity relationships around the scaffold were investigated, leading to the identification of compounds with IC_{50} values in the low micromolar range. One most active compounds (S009-2050) from this series inhibited PTP-1B with IC_{50} value of 8.32μM.This sulfonamide-based inhibitors exhibit significant improvement of random blood glucose as well as fasting blood glucose. Compound significantly improves the oral glucose tolerance test by 16.1 and 46.1% on 10th and 15th day post treatment compared to vehicle treated control group. Treatment of compound also improves the serum insulin level and HOMA index, a method used to quantify insulin resistance. Repeated oral gavages of compound improves the altered serum lipid profile which also contribute towards improved insulin sensitivity. Compound appears to regulate the muscular and hepatic insulin signaling and sensitivity in a similar manner to other phosphatases such as PTP1B, PTEN 1 by changing the phosphorylation status of the key members of the signaling pathway. mRNA analysis also reveals that treatment of compound results in significant upregulation and downregulation of IRS (I &II), Akt 2, PIK3CG, PTPN1 gene as all of them are involved in insulin signaling pathway.

PP-515

Studies on arene interactions: ^{1}H NMR and X-ray crystallographic studies with butylidene linker compounds

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ABSTRACT:

Arene-arene interaction or p–p interaction are known to play a key role in a wide range of important problems including the stereochemistry of organic reaction, host-gust chemistry, crystal packing, protein folding, DNA and RNA base stacking, protein-nucleic acid recognition and drug-receptor complex.[1] The p–p interaction is weak in strength with the energy ranging from 0-50 kj/mol but attractive interaction between two aromatic residues present in the same or different molecules.

These interactions have always been present in nature (e.g. in protein and DNA) but are less studied because of their weak and complex nature. Since 1995 our group has been working on flexible models of pyrazolo[3,4-*d*]pyrimidine for studying p–p interaction using *propylene* linker. Recently, we proposed *butylidene* linker as an alternative to *propylene* linker for studying arene interactions.[2] This linker is quite similar to *propylene* linker but somewhat less flexible which facilitates crystallization more easily than *propylene* linker. For example the compound **(1)** is based on purine shows intramolecular folding in solution by ^{1}H NMR analysis but this compound failed to crystallize. Corresponding compound **(2)** in which *propylene* is replaced by *butylidene* linker gets easily crystallized and folded conformation was confirmed by X-ray crystallography. Now we have synthesized models based on other biologically active nucleus rather than purines and pyrazolo[3,4-*d*]pyrimidine. The symmetrical dimer **(3)** based on benzotriazole was synthesized, however, both ^{1}H NMR analysis in solution and X-ray crystallography in solid state showed absence of intramolecular p–p interaction. This result indicates that benzotriazole with three N atoms as compared to four in purines and pyrazolo[3,4-*d*]pyrimidine may not be good system for studying intramolecular arene interactions in face-to-face (offset) mode.

PP-516
4-THIAZOLIDINONES: KEY INTERMEDIATES FOR FIVE-, SIX- AND SEVEN-MEMBERED HETEROCYCLES

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ABSTRACT

4-Thiazolidinone derivatives are the subject of renowned interest because they have been found to be useful intermediate for the synthesis of various heterocyclic compounds. 4Thiazolidinone derivatives occupy an important place in medicinal chemistry as they show a variety of pharmacological properties such as anti-convulsant, anti-HIV, anti-fungal, anti-bacterial, COX-1 inhibitor, anti-histaminic, anti-inflammatory, anti-fungal, anti-cancer, anti-tuberculostatic, anti-viral and diuretic properties.

It is evident from the strategy shown in scheme that 2-amino-5-aryl substituted 1, 3-thiazoles **(2a-d)** were required as the key intermediate in the execution of this plan. 2-amino-5-aryl substituted 1,3-thiazoles were prepared from phenacyl bromide **(1a-d)**. Treatment of 2-amino-5-aryl substituted 1,3-thiazoles **(2a-d)** with potassium thiocyanate yielded the corresponding thiazolyl thiourea **(3a-d)** in a good yield. Reaction of **(3a-d)** with $ClCH_2COOH$ furnished the 4-thiazolidinone derivatives **(4a-d).** The structures of all the compounds were established on the basis of their IR, HNMR and MS data. The exploration of biological activity of these materials is in progress.

PP-517
SYNTHESIS OF SOME NOVEL ISOFLAVONES USING DEOXYBENZOIN INTERMEDIATES AND EVALUATION ANTI-ANXIETY ACTIVITY

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ABSTRACT

Isoflavones are poly-hydroxy substituted 3-aryl-4*H*-chromen-4-ones which are found in the plant kingdom, mainly in legumes in the form of glycosides and aglycones. Isoflavones are structurally similar to mammalian oestrogen and oestradiol and have oestrogenic properties. These have remarkably diverse biological profile including osteoporosis, diabetes, cardiovascular and CNS. The isoflavones have been reported to possess antioxidant, anti-cancer, anti-cataracts, anti-inflammatory and anti-fertility activities. Various isoflavones and their derivatives were synthesized from deoxybenzoin intermediates **(3).** The deoxybenzoins were prepared from resorcinol **(1)** with the reaction of arylacetic acid **(2)** in the BF_3-Et_2O medium at 80^{o}C. The deoxybenzoins **(3)** were treated with methanesulphonyl chloride at 85^{o}C to obtain 6-ethyl substituted isoflavones **(4)** and acetic anhydride at 115^{o}C to produce 2-methyl-6-ethyl isoflavones **(6).** Compound **(4)** and **(6)** were then reacted with alkyl halides or aryl halides at room temperature to give corresponding alkylated or arylated products **(5)** and **(7).** Purity of all the synthesized compounds was checked by LCMS. The compounds synthesized were characterized with help of IR, ^{1}H NMR and MS spectral data. Biological properties of some of synthesized isoflavones have been screened at Pinnacle Biomedical Research Institute **(PBRI),** Bhopal (MP).

PP-518

ENOL ETHERS, CHALCONES, OXOKETENEDITHIO ACETALS AND DIMETHYL AMINOMETHYLENE KETONES OF QUINOXALINE: REACTIVE INTERMEDIATES TO SYNTHESIZE CARBAZOLES AND AZACARBAZOLES

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ABSTRACT

The enol ethers, chalcones, oxoketenedithio acetals and dimethyl aminomethylene ketones offer unprecedented opportunities to a chemist for the synthesis of a wide variety of heterocyclic materials. The ubiquitous presence of carbazoles, azacarbazoles, quinoxaline, pyrazoles and isoxazoles in a wide array of molecules exhibiting impressive biological properties has stimulated interest in the reviews, on the synthesis of their structural analogues where different constitution and biological activity could allow them to be used as novel chemotherapeutic agents. This aroused our interest in the synthesis of hetero ring fused quinoxalino condensed isoxazole, pyrazole, pyrimidines, carbazole and azacarbazole derivatives.

PP-519

OXIDATIVE TRANSFORMATION OF PROPANE-1-OL BY PYRIDINIUM CHLOROCHROMATE IN ACIDIC MEDIUM IN THE PRESENCE AND ABSENCE OF OXALIC ACID – A CATALYTIC EFFECT

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ABSTRACT

Kinetics of oxidation of propane-1-ol by pyridinium chlorochromate (PCC) has been studied in perchloric acid water medium in the presence and absence of oxalic acid. The reaction is first order with PCC when substrate alcohol or oxalic acid + alcohol are taken and absence of free radicals indicate that oxidation is neither one electron nor three electron. Effect of $[H^+]$ and ionic strength are also same in both the cases and product of oxidation is also the same.

Oxidation is first order with respect to alcohol similarly ΔK_{cat} also show first order but the energy of activation in greatly reduced in co-oxidation and this prove the catalytic property of oxalic acid and formation of an adduct which releases activation energy to a large extent and hence enhances the rate of oxidation very much.

PP-520

In vitro anti –dermatophytic activity of some plant essential oils from Assam.

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ABSTRACT

The present study was conducted to evaluate and establish the claim of antidermatophytic activities of four plant essential oils collected from various parts of Assam. Based on ethno medical knowledge in the use of plants essential oils against some common skin diseases in the area, an attempt has been made to assess the anti-dermatophytic property of these essential oils of plants against *Trichophyton rubrum, Trichophyton mentagrophytes, Trichophyton tonsurans, Microsporum gypseum* by inhibition zone agar cup diffusion method (1). MIC and MFC experiments are done according to standard procedure (2). In vitro results are very encouraging and are close to standard drugs.

PP-521
ISOLATION AND CHARACTERIZATION OF 3-O METHYL ELLAGIC ACID 4' -RHAMNOSIDE FROM THE STEM BARK OF *POLYALTHIA LONGIFOLIA* (SONN.) THW.

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ABSTRACT
The plant *Polyalthia longifolia* (Annonaceae) is an ornamental tree, that finds its reference in Indian medicinal literature owing to its popular hindi name Ashoka. In the traditional system of medicine the stem bark of *P. longifolia* has been used in various diseases and disorders like fever, skin diseases, diabetes, hypertension, helminthiasis, wound healing, diarrhea, scrofulous gland tumors and uterine disorders. The present study involves the isolation and characterization of 3-O-methylellagic acid 4'-rhamnoside from butanol fraction of hydroalcoholic extract of the stem bark of *P. longifolia*. The compound was isolated by different chromatographic techniques; purity was checked by TLC and HPLC and the structural ellucidation was done using various spectroscopic techniques viz. IR, ^{1}H NMR, ^{13}C NMR, DEPT (90 and 135), 2D NMR (COSY, HSQC, HMBC) and mass spectroscopy.

PP-522
One Pot Synthesis and antimicrobial studies of 2,4-diaryl-2,5-dihydro-1,5-benzothiazepine under microwave irradiation

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ABSTRACT
A new efficient and environmentally friendly green chemistry procedure for the synthesis of a series of 2,4-diaryl-2,5-dihydro-1,5-benzothiazepines 3a-j under microwave irradiation and solvent free conditions is described[1]. 1,5-benzothiazepines **3** have been synthesized by a microwave promoted one pot condensation of 2-aminothiphenol **2** and substituted chalcone **1** in the presence of basic solid support(anhy. K_2CO_3/ fused $Ba(OH)_2$) using N,N-dimethylformamide(DMF) as a reaction mediator[2,3]. The purity was determined using TLC and melting points and structural elucidations were carried out by spectral(IR, 1H-NMR, Mass) studies. The synthesized compounds were also used for various biological screening. Sulphur containing 1,5-benzothiazepines derivatives show good antibacterial and antifungal activity.

PP-524
Aza-Annulation on the 16-dehydropregnenolone, via tandem intermolecular Aldol process and intramolecular Michael addition with their DPP-IV inhibition activity

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ABSTRACT
Pregnenolone is a major hormone mainly present in human nerve tissues. Recent studies indicated that derivatives of pregnenolone have many profound activities, such as anti-inflammatory, anti-asthamatic, cytotoxic, antifeedant, lipid lowering, anti-viral and as inhibitors of testosterone 5a reductase which helps in the treatment of androgen sensitive prostate cancer in men. 16-Dehydropregnenolone acetate (16-DPA) finds increasing application as a versatile scaffold and building block for different steroidal drugs for it is an ideal platform for preparation of dexamethasone, *ß*-methasone, 5a-reductase inhibitor, and related other steroidal pharmacophores.
In the present study, we have synthesised substituted piperidine to ring D by applying Aldol condensation and Michael addition reaction. From this reaction, steroids with a new hexacyclic ring have been synthesized. They were evaluated as inhibitors of DPP-IV. The structures of compounds were confirmed by ^{1}H, ^{13}C, NMR and mass spectral analysis. Among seventeen compounds evaluated only five compounds **1**, **9**, **13**, **15** and **16** demonstrated significant inhibition of DPP-IV.

PP-525

Synthesis and antihyperglycemic evaluation of new 2-imino-4-thiazolidinone-5-carboxylic acids having pyrazolylpharmacophore

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ABSTRACT

Type I and Type II diabetes mellitus are now recognized as serious global health problem and growing rapidly world wide. Owing to the seriousness of Type II DM various pharmacological agents have been developed which include biguanidines, 2,4-thiazolidinediones etc. Metformin and pioglitazone are oral antidiabetic agents, used for the treatment of insulin-resistant overweight diabetes patients.

2,4-Thiazolidinediones (TZDs) are a group of pharmacological agents that enhance insulin action (insulin sensitizers) and promote glucose utilization in peripheral tissue. They significantly reduce glucose, lipid in rodent models of Type II DM and obesity. Pyrazoles are also emerged as potential antihyperglycemic agents. A number of pyrazolyl compounds have been cited in the literature and are found to elicit antihyperglycemic activity. The acidic functionality on the TZD ring is essential for its binding to PPAR?.

Literature survey reveals that there is scanty information on the molecules having pyrazoles, carboxylic acid and TZDs as their structural units. Considering the pharmacological importance of these above moieties and also the side effects associated with existing drugs, here new 2-imino-4-thiazolidinone-5-carboxylic acids having pyrazolyl moiety have been synthesized starting from readily available materials. The newly synthesized 2-imino-4-thiazolidinone-5-carboxylic acids have also been evaluated for their antihyperglycemic activity. The synthetic route is depicted in the following scheme. The details of the synthetic work and antihyperglycemic activity of the entitled products will be given in the presentation.

PP-526

Spectrophotometric determinations of Copper with 3-hydoxy-3-methyl-1-p-methoxy phenyl triazene

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ABSTRACT

3-Hydoxy-3-methyl-1-p-methoxy phenyl triazene has been established as a new reagent for determination of Copper. 3-Hydoxy-3-methyl-1-p-methoxy phenyl triazene has been prepared[1] (m.p. 80^0C) by coupling methyl hydroxylamine with diazonium salt in 1:1 molar proportion at 0-5^0C. The reagent solution was prepared in ethanol. The standard solution of copper was prepared by dissolving requisite quantity of copper sulphate pentahydrate (B.D.H., A.R.) in double distilled water. A few drop of concentrated H_2SO_4 were added to the solution to prevent hydrolysis. It was further standardized with EDTA using murexide as an indicator[2]. A systronics UV-VIS spectrophotometer-108 was used for spectrophotomrtric work and for pH-measurements systronics pH meter-324 was used. The green Cu (II) complex was soluble in ethanol and its color was stable for more than 24 h. It gives maximum absorbance at 380 nm but subsequent absorbances were made at 430 nm against solvent blank. Eight fold excess of the reagent was used and pH was kept between 6.0 to 6.6. The system obeys Beer's law in the range from15.88 ppm to 31.77 ppm of copper. Sandell's sensitivity is 47.4 ng/cm^2 and molar absorptivity is 2,040 liter/mole cm. The Job's method[3], Slope ratio method[4] and mole ratio methods- (i) Yoe & Jones[5] and (ii) Zolotov's[6] gave 1:2 (Fe:R) stoichiometery for the complex. Interference of 22 diverse ions was studied in determination of 31.77 ppm of copper. K(I), Cl^-, Br^-, SO_4^{--}, NO_3^- and CO_3^{--}, did not interfere when present in 100 ppm concentration. In addition to these ions, Na(I), NH_4^+, Br^-, CH_3COOH, and PO_4^{---} did not interfere when present in 50 ppm. The precision study was carried for 31.77 ppm of Cu (II), standard deviation was 0.03 ppm of copper. The solid complex was obtained as brown micro crystal, m.p. 158^0C with molecular formula Cu ($C_{14}H_{20}N_6O_4$). H_2O. This molecular formula corroborates the composition of the complex found with solution studies.

PP-527

Development of new method for Simultaneous determination of amlodipine with H1-receptor antagonists: Application in interaction studies

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ABSTRACT

Today, knowledge of cardiovascular drug interactions is regarded as basic to our understanding of the pharmacologic properties of these drugs. Such interactions can be either pharmacokinetic or pharmacodynamic. Many cardiovascular drugs are metabolized in liver, generally through the cytochrome oxidase system, involving one of several isoforms. Of the various isoforms, the CYP 3A4 is the site of most hepatic interactions of cardiac drugs. A number of interacting drugs and the herbal remedy can induce the CYP 3A4 isoform. Accordingly, such drugs accelerate the breakdown of those cardiovascular drugs that are metabolized by this isoform. Thus, the inducers lessen the blood concentrations of these drugs and their therapeutic efficacy. On the other hand, blood levels of these same drugs are increased by those agents that act as inhibitors of the CYP 3A4 isoform. Amlodipine is a long acting calcium channel blocker, used as an antihypertensive and in the treatment of angina. Antihypertension is a long term therapy. Co prescription of other drugs during this period can lead to drug interactions that could be lethal sometimes. Many of the interactions of calcium channel blocker are pharmacodynamic. H_1- receptor antagonists, often referred simply as antihistamines, are competitive inhibitor of histamine receptor H_1 and are used to treat allergies. Antihistamines are known to cause drug-drug interactions. Since antihypertension is a long term therapy, coadministration of amlodipine with antihistamines is possible and can lead to drug-drug interactions. Present study investigates possible changes in *in vitro* availability of amlodipine in presence of commonly used antihistamines like citrizine, levocitrizine, fexofinadine and buclizine were used in these studies. These studies were carried out in buffer of pH 4, 7.4 and 9 at 37 C° on B.P. dissolution apparatus 2007. Analysis was done using UV-Visible spectrophotometer and RP-HPLC. Mobile phase consisted of acetonitrile and phosphate buffer. The pH of mobile phase was maintained at 2.8. The flow rate was maintained at 1 ml/min. ? $_{max}$ for determination of interactions of amlodipine, citirizine and levocitrizine was 240nm and for amlodipine, buclizine and fexofinadine it was 230 nm. It was found that antihistamines studied bind to amlodipine and affect the therapeutic efficacy of these drugs.

PP-528

Chiral pool based synthesis of Polyhydroxylated Alkaloids by Using Diastereoselective Grignard Addition and Olefin Metathesis

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ABSTRACT

The saturated polyhydroxylated *N*-containing heterocycles, such as pyrrolidines, indolizidines, and pyrrolizidines have been shown to be potent inhibitors of a great variety of potent glycocidase[1] and also well-recognized for their chemotherapeutic potential as antibacterial, antidiabetic, antitumoral, and antiviral agents.[2,3] These polyhydroxylated alkaloids also known as iminosugars. Diverse activities of these compounds make them attractive to synthetic chemist in recent decades.[4]

Formal synthesis of three poly-hydroxylated alkaloids was carried out by using two important C-C bond forming reactions, Grignard reaction and olefin cross/ring closing metathesis[5] as the key steps from a common nitrone intermediate.[6] Commercially available sugars were used as a chiral pool material for the synthesis of highly functionalised nitrones.

PP-529

Photochromic behaviour of hexacyanoferrate(II) in phthalein and sulphophthalein system; a comparative study

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ABSRACT

The photochromic behaviour of hexacyanoferrate (II) and phthalein and sulphophthalein system was observed spectrophotometrically. Hexacyanoferrate (II) acts as a photo ejector. This ejected electron abstract H^+ from indicator molecule and respective molecule of the indicator changes into their quinonoud form,which is coloured. The effect of various parameters like PH, concentration of reactant, light intensity, etc, were observed on phtochromic behaviour shown by these system a tentative mechanism was proposed for this photochromic behavior.

INTRODUCTION : Photochromism is a light –induced reversible change of colour .Photochromic lenses are darken on exposure to ultraviolet radiation and return to their clear state in the absence of light. Establishment of a methodology for evaluation of photochromic textile using traditional colour measurement instrumentation [1].Synthesis and photochromism of tungstophosphate –functionalized ordered mesoporous hybrid silica[2] .photochromic behaviour of heaxacyanoferrate(II) phenolphthalein system by radha et.al[3] the present system describe the comparative study of photochromic behavior of hexacyanoferrate (II) in phthalein and sulphophthalein system.

PP-530

Microwave Assisted Synthesis of AZO Compound: A solvent free path for some new Sodium 4-[(2-hydroxyl-1-naphthyl) azo] benzene sulfonate derivatives and their antimicrobial activities

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ABSTRACT

An efficient one-pot synthesis of Sodium 4-[(2-hydroxyl-1-naphthyl)azo] benzene sulfonate has been achieved by the diazotized sulphanillic acid (1) coupling with ß-napthol in NaOH solution under microwave irradiation (MWI)[1] which then treated with conc. sulphuric acid, conc. sulphuric acid/ nitric acid + mecurus nitrate, ammonium sulphite and ammonia to give derivatives sodium -4 [(2-hydroxyl-8-sulfonapthalen-1-yl) diazenyl] benzene sulfonate (2a), sodium 4- [(2- hydroxyl-4-nitronatphalen-1-yl) diazenyl] benzene sulfonate (2b), sodium 4-[(2-aminonaphthalene-1-yl) diazenyl] benzene sulfonate (2c), under microwave irradiation and different catalyst used. All the products have been characterized by IR, Mass spectral analysis. Antimicrobial activities of these compounds were evaluated.

PP-531

MICROWAVE INDUCED SYNTHESIS AND CHARACTERIZATION OF ELECTROPHILIC SUBSTITUTED DERIVATIVES OF ANTHRAQUNONE DYES AND THEIR ANTIMICROBIAL ACTIVITY

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ABSTRACT

An efficient method for the one pot synthesis of 1,2,4-trihydroxy-3-nitro-9,10-anthraquinone, 1,-hydroxy-9,10-dioxo-9,10-dihydroanthracene2-yl-benzoate and 3-(ethoxycarbonyl)-4-hydroxy-9,10-dioxo-9,10 dihydroanthracene-2-sulphonic acid under microwave irradiation conditions. The structure of newly synthesized compounds have been established by analytical data includes elemental analysis, mass spectra, IR spectra and melting point.

❑❑❑

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