International Conference
on
"Expanding Horizons in Chemical and Biological Sciences: Innovations Crossroads"
ISCBC-2012

January 21st – 24th, 2012

ORGANIZED BY

School of Chemical Sciences,
Solapur University, Solapur
(Maharashtra)

UNDER THE AUSPICES OF

Indian Society of Chemists and Biologists

Lucknow

Prof. B. P. Bandgar
Vice-Chancellor,
Solapur University, Solapur

Message

I am indeed very glad that the 17th International Conference of the Indian Society of Chemists and Biologist under the theme "Expanding Horizons in Chemical and Biological Sciences: Innovations Cross-roads" ISCBC-2012 is organized by School of Chemical Sciences, Solapur University.

The Solapur University was established in 2004. Within a brief span of 7 years the university has taken significant strides towards excellence. From a humble beginning of three postgraduate departments, 50 affiliated colleges and about 60,000 students, now the university has seven schools with twenty-one postgraduate departments, 126 affiliated colleges with about 1,20,000 students from various faculties covering 240 academic programs at undergraduate, postgraduate and doctoral level. The university shone brilliantly in the field of sports and cultural events by bagging several honours at state and national level competitions. I am happy that now the academic departments are playing their role as evidenced by hosting this ISCBC-2012

The topics chosen for deliberation are of contemporary interest which include new methodology and technology for synthesis, nanotechnology, materials science in addition to drug design, drug delivery systems, bio and chemo informatics which warrant input from chemical as well as biological sciences.

A conference cannot be successful without eminent speakers and enthusiastic learners. I am glad leading researchers, academicians, professionals from abroad as well from various universities, research institutes and pharmaceutical companies from India will congregate at Solapur University to debate, deliberate to expand their sphere of research. Perhaps, the best part of the conference will be the opportunity to young scholars from this part of the world to intermingle with experienced and established researchers and imbibe the nectar of knowledge.

I heartily welcome the galaxy of scientists, academicians, professionals and delegates in this historic city of Solapur – Which is always warm even in winter, I wish all the success to the conference ISCBC-2012 and hope that some implementable recommendation will emanal from the conference.

Prof. Dr. B. P. Bandgar

Vice – Chancellor

Message from Organizers Desk

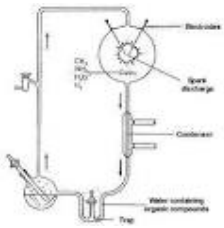
The Department of Chemistry was established in 1984 as one of the postgraduate department of Shivaji University Postgraduate Teaching Centre, Solapur. Since long it has been a cherished dream of all of us at the Department of Chemistry to organize a conference. We are happy that the dream is being realized now-as the 17th International Conference of the Indian Society of Chemists and Biologist on Expanding Horizons in Chemical and Biological Sciences. Innovation Crossroads" is organized to be held on 21st – 24th January, 2012. We are very much thankful to ISCB and particularly to Prof. Anamik Shah, President, ISCB and Dr. P.M.S. Chauhan, General Secretary, ISCB for giving us opportunity to organize this conference.

The topics for the deliberation for this conference transcend the borders of conventional Chemistry and biology and enter in the spheres of medicines, drugs, genetics, new synthesis methodologies, new materials including nonmaterial.

The tremendous advances in synthesis pathways coupled with the developments in biology and genetics has paved the way for more sustainable utilization of global resources. These development means that the pharmaceutical industry is well poised for explosive growth. Affordable health is a human right that can not be ignored and it is imperative that every individual not win standing his financial resources has access to new drugs. It is in this context that we feel the ISCBC-2012 is a step forward in the right direction.

There are 10 Plenary Lectures and 31 Invited Lectures in this conference. Apart from this there are 15 Oral Presentations and 176 Poster Presentations.

We welcome all the eminent academicians, scientists, professionals and research scholars from overseas as well as from all over India in this historic city of Solapur and hope that the deliberations



Prof. Anamik Shah
President & Organizing Secretary,
Indian Society of Chemists & Biologists

Message

I am privileged to welcome all the dignitaries, speakers from abroad and India and delegates from industries and academia at Solapur on behalf of Indian Society of Chemists and Biologists, Lucknow who spearheaded in organizing 17th International Conference on the focal theme "Expanding Horizons in Chemical and Biological sciences: Innovations Crosswords" jointly with Solapur University under the able leadership of Hon'ble Vice Chancellor B.P. Bandgar. The founders of Indian Society of Chemists and Biologists, Lucknow has envisioned the importance of amalgamation of chemical and biological sciences in 1995 and I am very happy to note that this fact has now been universally accepted in last decade and therefore ISCB is receiving overwhelming support from interdisciplinary and multidisciplinary sciences for meaningful get together and discuss various branches/subjects like chemistry, biology, biochemistry, medicinal chemistry, pharmaceutical sciences, nanotechnology and biotechnology.

The roadmap for Indian Science and especially health science is concerned; the country has to play a vital role for affordability of medicines for all. National Innovation Council's recent report also gives future directions in this area. I am very happy that the objective of this conference is to bring together students, researchers, scientist and academicians from various fields on a common platform to share the knowledge, experience and expertise for betterment of mankind.

On behalf of ISCB office bearers, I take this opportunity to congratulate the entire 17th ISCB-2012 team, especially Prof. S.V. Lonikar, Dr. Anil A. Ghanwat, Prof N.N. Maldar and Prof. P.G.More for their dedication and hard work to make this event a memorable one. I hope that delegates especially students delegate will get a true spirit of vibrancy by this conference their future endeavor. I also appeal to all delegates to join ISCB as life members to enjoy such wonderful happenings every year in different part of India. I wish a grant success to this conference.

(Prof. Anamik Shah)
President, ISCB

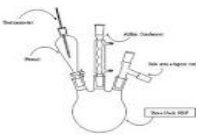
Dr. P.M.S. Chauhan
General Secretary
Indian Society of Chemists & Biologists

Message

Interdisciplinary interactions of researchers are of prime importance for the advancement of knowledge and applications of knowledge. Such interactions are much more important when come to drug research. However the process of drug research has become more difficult, risky and expensive due to very tight regulatory parameters. To make a break through in this area a close interaction between the scientists and technologists in the area of chemistry and biology is highly desired. With this view in mind Indian of Society Chemists and Biologists is making consistent efforts to encourage interdisciplinary research activities in the field of chemistry and biology. Indian Society of Chemists and Biologists is unique in the sense that it promotes multidisciplinary research as compared to several scientific societies in the individual capacity with confined objectives. During the past the society has been very successful in achieving the targets. We are extremely happy 17th International Conference on "Expanding Horizons in Chemical and Biological Sciences: Innovations Crossroads" to be held at Solapur University, Solapur, We are glad that the scientific committee is bringing out an abstracts book covering the presentation to be made during ISCBC-2012. 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 8 plenary lectures, 27 invited lectures by the eminent scientists from India and abroad, 22 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 Solapur.

PMSchauhan

(Dr. P.M.S. Chauhan)



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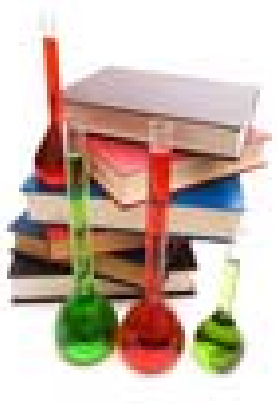

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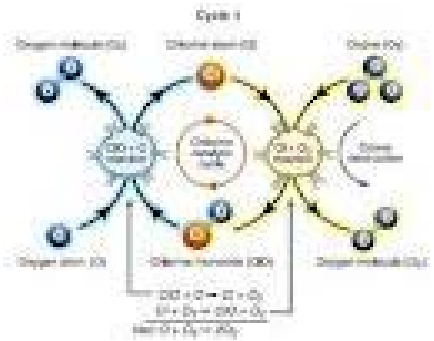

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ISCBC - 2012,

Solapur University, Solapur

21 JANUARY 2012, DAY 1st		
03:00-04:00 pm	**INAUGARAL FUNCTION : ISCBC-12**	
04:00-04:20 pm	TEA BREAK	
Session I : 04.20 pm – 06:20 pm **Session Chair : Professor Peter A. Beal**		
04:20-04:50 pm	PL 1.	Aspects of Chemical Biology of Carba – LNA modified Oligos formRNA Targeting Prof. Jyoti Chattopadhyaya, Program of Chemical Biology, Dept. of Cell & Molecular Biology, Uppsala University,
04:50-05:20 pm	PL 2.	Discovery of novel HDAC and G-quadruplex stabilization compounds from Natural and non-natural sources Srivari Chandrasekhar Indian Institute of Chemical Technology, Hyderabad, India.
05:20-05:50 pm	PL 3.	Trends and Perspectives of Applying of Natural and Synthetic Aporphinoid Alkaloids Prof. Sergey F. Vasilevskiy Institute of Chemical Kinetics and Combustion of Siberian Branch, The Russian Academy of Sciences, Russia
05:50-06:20 pm	PL 4.	Towards the total synthesis of bioactive indole alkaloids Dr. Dattatraya Dethe IIT, Kanpur.

22 JANUARY 2012 DAY 2nd		
Session II : 09.00 am – 10:40 am **Session Chair : Professor Sergey F. Vasilevskiy**		
09:00-09:30 am	PL 5.	Formation of N^3 – alkylquinazolin-4-ones and 1-alkoxyquinazolines from anthranilamides and orthoamides Prof. Mike Threadgill Bath University, UK

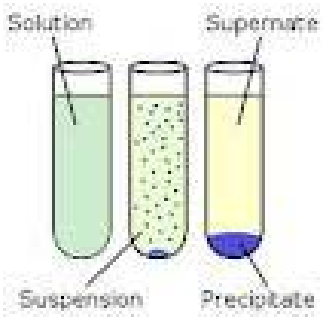
09:30-10:00 am	PL 6.	On the Diastereoselective Oxidation of 8-(4-Bromophey1)-8ethoxy-5methyl- 8H[1,4]thiazino[3,4-c][1,2,4] oxadiazol-3-one: a Combined Experimental and Computational Investigation Prof. Domenico Spinelli, Italy
10:00-10:20 am	IL1.	Drug Discovery and Development from Medicinal Plant-derived Natural Products: Recent Trends and Opportunities for India. Dr. Sanjay M. Jachak Associate Professor Department of Natural Products National Institute of Pharmaceutical Education and Research (NIPER) Mohali.
10:20-10:40 am	IL 2.	The role of water in C-N, C-S and C-O bond forming reactions in organic synthesis Prof. V.K.Tandon, Dean of Science Faculty, Lucknow university.
10:40-11:15 am	TEA BREAK	
Session III : 11:15- 01:15pm **Session Chair : Dr. P.T.Perumal**		
11:15-11:35 am	IL 3.	Synthesis of biologically active Natural products from carbohydrate building blocks Dr. A.K. Shaw Medicinal and Process Chemistry Division CSIR-Central Drug Research Institute, Lucknow.
11:35-11:55 am	IL 4.	Stereoselective Synthesis of Biologically Active Azacyclic Compounds: Prof. Sundarababu Baskaran Department of Chemistry, Indian Institute of Technology Madras, Chennai.
11:55- 12:15 pm	IL 5.	Tetraoxane and amino-quinoline scaffold based hybrids: Synthesis and antimalarial activity Evaluation Prof. Diwan Singh Delhi University, Delhi.
12:15- 12:35 pm	IL 6.	Design and Synthesis of Azaheterocycles as Novel Antitubulin Agents Dr. Dalip Kumar BITS, Pilani.

12:35-12:55 pm	IL 7.	Pyrazolo[3,4-d] pyrimidine core based models for studying II-II interactions in flexible propylene and butylidene linker compounds at molecular and supramolecular level Dr. K. Avasthi Medicinal and Process Chemistry Division CSIR-Central Drug Research Institute, Lucknow.
12:55-01:15 pm	IL 8.	Backbone Modified Nucleic Acids and Sugar- PEG Based Polymeric Architecture of Importance Prof. Ashok Prasad Delhi University, Delhi.
01:15- 02:15 pm	LUNCH BREAK	
Session IV : 02:15- 03:35pm **Session Chair : Dr. P. P. Wadgaonkar**		
02:15- 02:35 pm	IL 9.	Polymorphism in Pharmaceuticals and Intellectual Property Dr. U. P. Sinthilkumar Orchid Research Laboratories Limited, Chennai.
02.35- 02:55 pm	IL 10.	Green Chemistry:Basic principles & Atom Economy B. Gopalan, Ph.D, CSO, Drug Discovery Research, Orchid Research Laboratories Limited, Chennai.
02.55- 03:15 pm	IL 11.	The Art and Science of Crystallization in Active Pharmaceutical Industry (API) Dr. R.J. Sarangdhar Orchid Research Laboratories Limited, Chennai.
03.15-03:35 pm	IL 12.	Prof. K. S. Rangappa Vice-Chancellor, Karnataka State Open University,
03.35- 05:35 pm		AWARD SESSION
03:35-04:05 pm		Prof. Jyoti Chattopadhyaya ISCB AWARDS FOR EXCELLENCE-2012
04:05-04:20 pm		Dr.KARUNAKARAN Venugopal ISCB Young Scientist Award
04:20-04:35 pm		Dr.Latha Rangan ISCB Young Scientist Award
04:35-04:50 pm		Dr.Girish Mahajan ISCB award of appreciation for industry scientist
04:50-05:05 pm		Dr.Sanjay Kumar ISCB award of appreciation for industry scientist
05:05-05:20 pm		Dr.Rakeshwar Bandichhor ISCB award of appreciation for industry scientist
05:20-05:35 pm		Dr.Janapala Venkateswara Rao – Dr. Vinod Bhakuni memorial ISCB award
	TEA BREAK	
02:15-06:30 pm	**Poster Presentation Session**	

23 JANUARY 2012 DAY 3rd		
Session V : 09:00- 10:50 am **Session Chair : Prof. Mike Threadgill**		
09:00-09:30 am	PL 7.	New Organocatalysts for the Asymmetric Allylation and Reduction Prof. Pavel Kocovsky, FRSE Department of Chemistry University of Glasgow Glasgow G12 8QQ, UK
09:30-10:00 am	PL 8.	Chemistry and Biology of the Repair of Oxidized Guanines Prof. Sheila S. David University of California Davis Davis, CA 95616, USA
10:00-10:20 am	IL 13.	Branching Cascades in Diversity Oriented Synthesis Dr. Nitin Patil Senior Scientist, Organic Chemistry Division – II Indian Institute of Chemical Technology; Hyderabad.
10:20-10:40 am	IL 14.	Carbocyclic and heterocyclic compounds synthesis from alkynes and nitriles Prof. P.T. Perumal, Chief Scientist & Head Organic Chemistry Division, Central Leather Research Institute, Chennai-600020.
10:40-10:50 am	OP 1.	Mr. Amol G. Patne Ph. D. Scholar, Universita Roma Tre, via della Vasca Navale, Roma, Italy
10:50-11:15 am	TEA BREAK	
Session VI : 11:15- 01:15 pm **Session Chair : Dr. Abhijit Roychowdhury**		
11:15-11:35 am	IL 15.	Remarkably Selective Nucleophilic Reactions of Cyclic Anhydrides and Derivatives: Synthesis of Nitrogen Containing Bioactive Natural Products Dr. Narshinha P. Argade National Chemical Laboratory (CSIR), Pune.
11:35-11:55 am	IL 16.	Pantolactone Chiral Pool Approach: Synthesis of Bio-active Natural Products Dr. Srinivas Reddy, National Chemical Laboratory, Pune.

11:55-12:15 pm	IL 17.	Role of Biomedical Imaging in Modern Drug Discover Dr. Datta Ponde Director, Deccan Institute of Chemical Technology, Jogging Park, Savedi, Ahmednagar.
12:15- 12:35 pm	IL 18.	Dr. M.M.V. Ramana Professor of Organic Chemistry, Department of Chemistry, University of Mumbai.
12:35- 12:55 pm	IL 19.	Prof. B. Kesava Rao Head Dept. of Chemistry, University College of Sciences, Acharya Nagarjuna University, Nagarjunanagar.A. P.
12:55- 01:15 pm	IL 20.	Dr. Bhawani Singh Department of Chemistry Banasthali University, Banasthali (Rajasthan)
01:15- 02:15 pm	LUNCH BREAK	
Session VII : 02:15- 04:15 pm **Session Chair : Dr. Narshinha P. Argade**		
02:15- 02:35 pm	IL 21.	Natural product scaffold based lead optimization against Tropical neglected diseases Dr.Harish Holla Griffith University, Don Young Road, Nathan Brisbane, Queensland 4111, Australia.
02:35-02:55 pm	IL 22.	Enabling Green Chemistry and Profitability through Effective Process Research Dr. Dhillep Krishnamurthy, Dr. Reddy's Laboratories Ltd. Hydrabad.
02:55-03:15pm	IL 23.	Toxicophores in Drug Discovery Dr. Abhijit Roychowdhury Piramal Life Sciences Limited, Goregaon (E), Mumbai.
03:15-03:35 pm	IL 24.	Designing Specific Drugs By Disrupting Interaction between Preformed Signaling Complex of Inactive G-Proteins and Adenylyl Cyclase Isoforms Dr. Rachna Sadana Biology and Biochemistry Department 1 Main St, N609 UH-Downtown Houston, TX, USA
03:35-03:55 pm	IL 25.	Design, synthesis, and biological evaluation of DGAT1 inhibitors as potential anti-obesity agents Dr. Amol Gupte Piramal Life Sciences Limited, Goregaon (E), Mumbai.

03:55-04:05 pm	OP 2.	D. N. Singh Department of Chemistry, K.S. Saket PG College, Dr. RML Avadh University, Faizabad.
04:05-04:15 pm	OP 3.	Dr. Malay K. Das Dibrugarh University, Dibrugarh.
04:15-04:45 pm	TEA BREAK	
Session VIII : 04:45-05:45 pm **Session Chair : Dr. Dattatraya Dethe**		
04:45-05:05 pm	IL 26.	" Enzymes as an attractive tool for Chemical transformations " Dr. Keshav Deo Vice President - CRD Wockhardt Research Centre # D-4, MIDC, Ind.Area, Aurangabad - 431210, INDIA
05:05-05:15 pm	OP 4.	Dr. P. Thirupathi Department of Chemistry; 5E 414 B, Bioorganic Chemistry Laboratory; Inha University, 253 Yonghyun-Dong, Nam-Gu; Incheon, South Korea.
05:15-05:25 pm	OP 5.	Dr. Suniti Dharwadkar S.B. College of Science Auranagabad.
05:25-05:35 pm	OP 6.	V. Badireenath Konkimall FC 210; School of biological sciences National Institute of Science Education and Research (NISER; Institute of Physics Campus, Sachivalaya Marg, PO:Sainik School, Bhubaneswar.
05:35-05:45 pm	OP 7.	Vivek T. Humme Department of Chemistry, Institute of Chemical Technology, Matunga, Mumbai.
05:00-06:30 pm	**Poster Presentation Session**	



24 JANUARY 2012 DAY 4th		
Session IX : 09:00- 10:50 am **Session Chair : Prof. Pavel Kocovsky, FRSE**		
9:00-09:30 am	PL 9.	Nucleic Acid Chemical Biology: Studies in RNA interference and RNA editing Prof. Peter A. Beal Department of Chemistry University of California Davis Davis, CA95616,USA
09:30-10:00 am	PL 10.	Peptides as potential biomarkers for medical diagnostics Prof. Vadim T. Ivanov Russian Academy of Sciences Shemyakin & Ovchinnikov Inst. Of Bio. Chem. UI. Miklukho-Maklaya, Russia.
10:00-10:20 am	IL 27.	Sulfur and Nitrogen Containing Bisphosphonic Acids are a corner stone for Calcium- Related Disorders and their Role in Oncology Dr. Wafaa Abdou, Professor of Applied Org. Chem.(Mrs,D.Sc.), National Research Centre, Cairo, Egypt.
10:20-10:30 am	OP 8.	Mr. Sidhendra Kupal Departimento di Scienzee Tecnologie Chemiche, Universita ' di Roma " Tor Vergata", Via Della Ricerea Scientifica, Roma, Italy.
10:30-10:40 am	OP 9.	Anand S. Burange Department of Chemistry, Institute of Chemical Technology, Matunga, Mumbai.
10:40-10:50 am	OP 10.	Dr. Archana Taunk Chemistry Dept, R D National college Linking rd, Bandra west, Mumbai.
10:50-11:15 am	TEA BREAK	
Session X : 11:15 am - 01:25 pm **Session Chair : Dr. S. Bhaskarn**		
11:15-11:35 am	IL 28.	Macromers as Targeted Nano Delivery Materials: Opportunities and Challenges Dr. Jayant Khandare Piramal Life Sciences Limited, Goregaon (E), Mumbai.

11:35-11:55 am	IL 29.	Perspectives and Challenges in Drug Research: Design and Synthesis of Nitrogen Heterocycles as Novel therapeutic Agents Dr. P.M.S. Chauhan Medicinal and Process Chemistry Division CSIR-Central Drug Research Institute, Lucknow.
11:55- 12:15 pm	IL 30.	Structure & Scaffold Based Synthesis of Heterocycles as Favored Pharmaceuticals: Bioevaluation Dr. V. Jaiteerth Rao, Indian Institute of Chemical Technology, Hyderabad.
12:15-12:25 pm	OP 11.	R. I. Kureshy Discipline of Inorganic Materials and Catalysis, Central Salt and Marine Chemicals Research Institute (CSIR-CSMCRI), Bhavnagar, Gujarat.
12:25-12:35 pm	OP 12.	S. K. Borthakur Department of Chemistry, Arya Vidyapeeth College, P.O. Gopinath Nagar, Guwahati, Assam.
12:35-12:45 pm	OP 13.	Pradeep K. Srivastava Principal Scientist, Medicinal & Process Chemistry Division CDRI, Lucknow
12:45-12:55 pm	OP 14.	N. H. Khan Discipline of Inorganic Materials and Catalysis, Central Salt and Marine Chemicals Research Institute (CSIR-CSMCRI), Bhavnagar, Gujarat.
12:55-01:05 pm	OP 15.	Indresh Kumar Organocatalytic Direct Aldol Reaction: Green approach towards the synthesis of Amino-Polyols Shri Mata Vaishno Devi University, Katra (J & K)
01:05 –01:25 pm	IL 31.	Approaches towards design and synthesis Anticancer Agents Prof. Anamik Shah Principle Investigator: "National Facility for Drug Discovery through New Chemical Entities(NCE's) Development & Instrumentation Support to Small Manufacturing Pharma Entrprises" Department of Chemistry, (UGC-SAP & DST-FIST funded) Saurashtra University, Rajkot-360005 (INDIA)
01:25-02:30 pm	LUNCH BREAK	
02:30-03:45 pm	**Valedictory Function**	

Prof. J. Chattopadhyaya (University of Uppsala, Sweden)

Professor Jyoti Chattopadhyaya is a Chair of Bioorganic Chemistry and is also Program Director of the Chemical Biology Program 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 1979, and since than he has supervised research of 30 Ph.Ds and promoted 3 D.Sc (Docents). He has published original multidisciplinary research in the interface of Synthetic and Physical chemistry, Structure by NMR, Enzymology and Molecular biology resulting in over 410 publications in various peer-reviewed Journals (for details see http://www.boc.uu.se). Prof. Chattopadhyaya's research focuses on the design of *gene (RNA)-directed therapeutics from design and synthesis to Biology*. He was awarded with Norblad-Ekstrand Gold Medal (1993) by Swedish Chemical Society, Humboldt Research Prize (1995) from Alexander von Humboldt Stiftung, Germany. The Sorm award (2007/8) from Czech Academy of Sciences. The Sorm Lectureship (2007/8) from Czech Academy of Sciences. He was awarded Visiting Professor (1995-'96) as a Humboldt Research Prize Winner at the Dept of Organic Chemistry at the Technical University of Munich, D-85747 Garching, Germany. He is also a Guest Professor (2003-) at the Dept of Organic Chemistry at the Jilin University, Changchun, 130012 China, as well as of Nankai University (Sep 2010-) at the College of Chemistry, Tianjin. He is a member of Editorial boards of over 11 international Journals. ISI Web of knowledge Citation Report: Results found: 350; *Sum of the Times Cited*: 6111; *Sum of Times Cited without self-citations*: 4243; A*verage Citations per item*: 17.46; *H-index*: 36. "Placed in the top 5% of the cited authors for Journals in Chemistry" - quoted by American Asthma Foundation, SF, Calif, USA. Oct 2011.

PL 1

ASPECTS OF CHEMICAL BIOLOGY OF CARBA-LNA MODIFIED OLIGOS FOR MRNA TARGETING

Jyoti Chattopadhyaya

Program of Chemical Biology (ICM), Box 581,

Biomedical Centre, Uppsala University, SE-75123 Uppsala, Sweden

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Fine tuning of the electrostatic properties around the internucleotidic phosphate can be achieved by in-corporations of lipophilic *vs* hydrophobic substituents on the Carba-LNAs and –ENAs leading to significant modulation of the antisense and small interferring RNA (siRNA) properties, such as target affinity, nucle-ase resistance and RNase H or the ago protein elicitation. This study, with synthetic chemistry, enzymology and NMR structure, gives an insight on the importance of chemical characters of the substituent-type in the carbocyclic moiety of carba-LNA and carba-ENA in the minor groove for the design of the RNA targeted therapeutics.

Upon screening of 52 modified antisense oligonucleotides, containing 13 differently functionalized car-ba-LNA/ENA derivatives, two excellent modifications have been found, which facilitate excellent target RNA affinity, nuclease resistance and RNase H activity, and they are deemed to be excellent candidates as potential antisense and siRNA therapeutic agents against target mRNA.

This study finally shows how the appropriate RNA target selection in the HIV genome and their specific inhibition by the siRNA approach by the choice of appropriate chemistry can also successfully modulate the expression and inhibition of HIV-specific proteins. In summary, We will discuss here the key role of inno-vative chemistry responsible in steering of the biological function (Chemistry-Biology interplay).

Speaker thanks Swedish Research Council (VR) and EU Framework programs for funding of this research, and also thanks all cited authors for their excellent contributions

Dr. S. Chandrasekhar, FNASc., FASc
Chief Scientist,
Organic Chemistry Division I, Indian Institute of Chemical Technology, Hyderabad - 500 007
srivaric@iict.res.in

Dr Srivari Chandrasekhar has made significant contributions in diverse areas of organic chemistry especially in chiral chemistry and total synthesis of biologically active natural products (marine natural products with architectural complexity). The design of new molecular entities, hybrid natural products, peptides involving unusual amino acids as defined foldamers is well received globally. The development of PEG as novel solvent medium created a totally different platform for practitioners of Green chemistry. Development of new methodologies for C-C bond formation reactions involving organo-catalysis and organo-metallic reagents is highly cited. The collaborative projects in applied areas of pharmaceutical research for both process development and drug discovery have resulted in development of economically viable processes and also several lead compounds for further optimization. To his credit he has 205 publications and two patents with over 3300 citations. 25 students have already obtained their Ph.D. award under his able guidance and 25 students are currently pursuing their research work with Dr. S. Chandrasekhar towards the Ph. D. programme.

He is the recipient of the Natioanl Academy of Sciences-Reliance platinum jubilee award in physical sciences for relevant work on innovations in applied research with fundamental approach. He has been awarded the Ranbaxy Research award in Pharmaceutical sciences for the year 2009 for his contributions to total synthesis of natural products and medicinal chemistry. He is fellow of the Indian Academy of Sciences and National Academy of Sciences.

Dr. Srivari obtained his Bachelors, Masters and Ph. D. degree from Osmania University while the work for Ph. D. was carried out in IICT on total synthesis of Cyclosporin. He was Alexander von Humbodlt Fellow at Goettingen and post-doctoral fellow at University of Texas.

PL 2

DISCOVERY OF NOVEL HDAC AND G-QUADRUPLEX STABILISATION COMPOUNDS FROM NATURAL AND NON-NATURAL SOURCES

Srivari Chandrasekhar

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Bioorganic & Medicinal Chemistry Letters, Volume 22, Issue 1, 1 January 2012, Pages 645-648

Srivari Chandrasekhar, Sreerangam N.C.V.L. Pushpavalli, Srinivas Chatla, Debasmita Mukhopadhyay, Bogonda Ganganna, Kandi Vijeender, Pabbaraja Srihari, Chada Raji Reddy, M. Janaki Ramaiah, Utpal Bhadra

Both marine and terrestrial organisms have played a prominent role in providing novel natural products as potential drugs. Our group is engaged in the synthesis of these natural products. The present lecture will highlight some of our recent contributions in this area. The total synthesis of cyclic peptide natural product Azumamide, non natural cyclic and acyclic peptides and their mimics will be described. The biological screening of these compounds in cancer therapy especially as novel HDAC inhibitors and G-quadruplex stabilisation will also be presented.

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Prof. Sergey F. Vasilevskiy

Head of Laboratory of Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia AWARDS - Honorary Inventor of USSR. Medal of Int. Biographic Center, Cambridge "2000 Outstanding Scientists of XX Century". Gold Badge and Diploma for scientific achievements and International scientific collaboration of International Philanthropy Society "Scientific Partnership"

VISITING PROFESSOR -

Heidelberg University, Germany 1993.

Ecole Normale Superieure, Paris, France, 1993,

Utrecht University, Holland 1991.

Cardiff University, England, 2001.

Madrid Institute of Medical Chemistry, Spain, 2001.

Thessaloniki Univ., Greece, 2006.

AREA OF SCIENTIFIC INTERESTS - The development of the methods of syntheses of aryl- and hetarylacetylenes with application of transition metal catalysis. The study of the structure-reactivity relationship of functional acetylenes. Supramolecular chemistry.

Modification of natural products and investigation of biological properties.

PUBLICATION - Total amount of publications about 200 (4 reviews)

THE BOOK - L.Brandsma, S.F.Vasilevsky, H.D.Verkruijsse "Application of Transition Metal Catalysts in Organic Synthesis" Springer-Verlag, Heidelberg, Berlin, New- York. 1998, 335p.

E-mail: vasilev@kinetics.nsc.ru http://www.kinetics.nsc.ru/spac/welcom.htm

PL 3

TRENDS AND PERSPECTIVES OF APPLYING OF NATURAL AND SYNTHETIC APORPHINOID ALKALOIDS

Sergey F. Vasilevskiy, Denis S. Baranov

Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, 630090, Novosibirsk, Russian Federation.

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Aporphinoid alkaloids are an important group of plant secondary metabolites. More than 500 aporphine alkaloids have been isolated from various plant families and many of these compounds possess potent DNA binding affinity, cytotoxic and antitumor activities [1-3].

. Here we review origin, synthesis, structure and biological properties of this promising class of compounds. This review presents discussing about the role of synthetic approach to Aporphinoid alkaloids for the systematic search of new medicinal agents.

Just last decade is noted by increasing interest to the applications of innovative synthetic methods for accelerated search of new medicinal agents.

We have developed a new one-step synthesis of 2-R-7H-dibenzo[de,h]quinolin-7-ones – compounds related to Aporphinoid family from 1-R-ethynyl-9,10-anthraquinones with a wide selection of functional groups and some polyfunctional N-containing reagents.

In report are given some new reactions and rearrangements, suggested possible mechanisms of these transformations, showed dependence of direction of reactions from internal and external factors.

Acknowledgements

This work was supported by Grant RFBR No. 10-03-00257-a (2010-2012), “Integration” program Grant of SB of the Russian Academy of Sciences (2012-2014) and the Chemical Service Centre of SB RAS.

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Dr. DATTATRAYA H. DETHE

Assistant Professor
Department of Chemistry
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Email: ddethe@iitk.ac.in

ACADEMIC QUALIFICATION:

Doctor of Philosophy (Organic Chemistry) 1999-2005
Department of Organic Chemistry
Indian Institute of Science, Bangalore, India.

RESEARCH EXPERIENCE

Post-Doctoral Research:

Research Supervisor: Prof. K. C. Nicolaou (Aug. 2005-July 2008)

1. Completed the first total synthesis of thiopeptide antibiotic natural products GE2270A, GE2270C1 and GE2270T using hetero Diels-Alder dimerization reaction and one pot tandem macrocyclisation as key steps.

2. Completed first total synthesis of natural products Amythiamicin A, B and C

3. Synthesized numerous analogues of anticancer natural product Palmerolide A biological screening, some of which has exhibited 10 fold increase in potency from that of natural product Palmerolide A.

4. Completed formal synthesis of Platencin.

Career: Dec 2011-Assistant Prof., Dept. of Chemistry, IIT Kanpur
July 2009 – Nov 2011, Scientist 'E-I', Organic Chemistry Division, National Chemical Laboratory, Pune, India.
July 2008 – July 2009. Senior Research Scientist, Drug discovery and Development Department, Albany Molecular Research Inc., Singapore.

AWARDS AND SCHOLARSHIPS

1. CSIR young scientist award for year 2011
2. Young associate of Indian academy of sciences Bangalore 2011-2014
3. OPPI Young Scientist award for year 2011.

RESEARCH INTERESTS

Total Synthesis of Natural Products.
Development of New Synthetic Methodologies
Drug Design and Development.

PL 4

TOWARDS THE TOTAL SYNTHESIS OF BIOACTIVE INDOLE ALKALOIDS

Dr. Dattatraya Dethe,

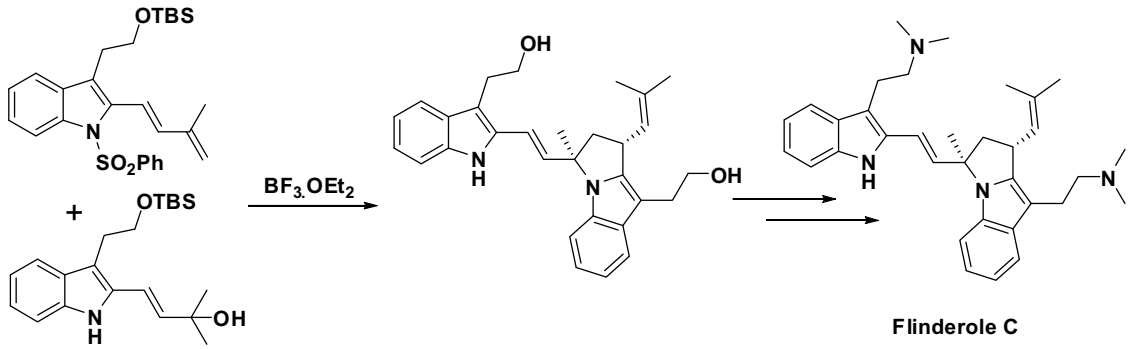
Assistant Professor

Dept. of Chemistry, IIT Kanpur.

ddethe@iitk.ac.in

Flinderoles A, B and C were Isolated from the Australian plant *Flindersia acuminata* in 2009, and Found to have selective antimalarial activities with **IC50** value **150 nm**. Here we have developed a highly regio- and stereoselective formal [3+2] cycloaddition reaction between a tertiary alcohol and an olefin for the synthesis of pyrrolo [1,2-a]indoles. Various Lewis acids were screened for the proposed dimerization of which $BF_3.OEt_2$ was found to be a useful catalyst for effecting this transformation in a much cleaner manner. In order to expand the scope of the reaction, several diverse examples were carried out and the potential of this methodology has been amply demonstrated by the first total synthesis of the isomeric flinderoles B and C, which involves 11 steps in the longest linear sequence and gave an overall yield of 17.2%. The strategy is fairly general and is amenable to the synthesis of other class of natural products borreverines, as well as their analogues.

Total Synthesis of Flinderoles B and C :-



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Professor Michael D. Threadgill

Professor Mike Threadgill gained his MA in the Natural Sciences Tripos from the University of Cambridge in 1974. He then trained as a teacher at the University of Durham, being awarded the Postgraduate Certificate in Education in 1975. During the following period (1975-1977) in medicinal chemistry research with Hoffmann-La Roche Ltd., he realised that his career would progress only with a PhD, so he joined the research group of Professor Sir Alan Battersby FRS at the Lensfield Road Chemical Laboratories of the University of Cambridge in October 1977. He completed his thesis "Synthetic studies related to cytochrome oxidase", working on assembly of □,□-linked cofacial bisporphyrins, and was awarded his PhD in 1981.

He was then attracted to the rapidly developing interdisciplinary cancer research group at Aston University, Birmingham and worked there as a Research Fellow until 1987. This period confirmed his interest in medicinal chemistry, drug discovery and drug metabolism. From here, he moved to his first formally independent position at the Medical Research Council Radiobiology Unit to lead a small medicinal chemistry team. In 1990, he was invited to join the University of Bath as a Lecturer in Medicinal Chemistry in the School of Pharmacy & Pharmacology. At Bath, he has developed his research in the medicinal chemistry of cancer, ischaemia-reperfusion diseases and tuberculosis, focussing particularly on inhibitors of the poly(ADP-ribose) polymerases, on heterocyclic chemistry and on the medicinal chemistry of boron clusters. He was promoted Senior Lecturer in 1993, Reader in 2000 and Professor in 2008 and is now Head of Medicinal Chemistry and University Ombudsman for Postgraduate Research Students. Thirty postgraduate research students have obtained PhD or MPhil under his supervision and he has published 130 research papers.

PL 5

FORMATION OF N^3-ALKYLQUINAZOLIN-4-ONES AND 1-ALKOXYQUINAZOLINES FROM ANTHRANILAMIDES AND ORTHOAMIDES

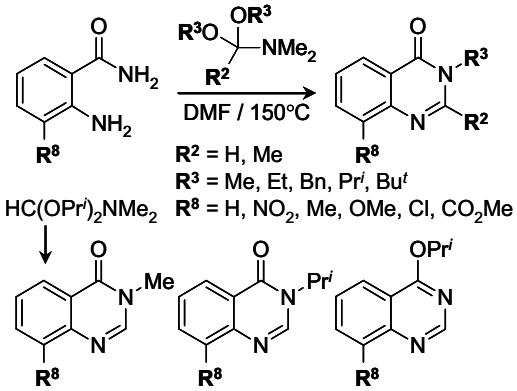
Michael D. Threadgill,* Amit Nathubhai, Richard Patterson, Timothy J. Woodman, Harriet E. C. Sharp, Miranda T. Y. Chui, Hugo H. K. Chung, Stephanie W. S. Lau and Jun Zheng

Medicinal Chemistry, Department of Pharmacy & Pharmacology, University of Bath, Claverton Down, Bath BA2 7AY, UK

m.d.threadgill@bath.ac.uk

Tankyrases-1 and -2 are members of the poly(ADP-ribose)polymerase (PARP) family of enzymes and have emerged recently as important targets for drug design for treatment of cancer.[1] 5-Aminoisoquinolin-1-one (5-AIQ) is a moderately potent but water-soluble and bioavailable inhibitor of PARP-1, with many potentially useful activities *in vitro* and *in vivo*.[2-4] Using 5-AIQ as template, we proposed 8-substituted quinazolin-4-ones as inhibitors of PARPs and tankyrases, as the N^3-H compounds contain the required lactam. Reaction of 3-substituted anthranilamides with dimethylformamide dimethylacetal (DMFDMA) at 150°C for very short periods gave mainly quinazolin-4-one.[5] Prolonged reaction with DMF di(primary-alkyl)acetals led to alkylation at N^3. The source of the N^3-alkyl group is the orthoamide O-alkyl. Reaction with the more sterically encumbered DMF di(isopropyl)acetal diverts alkylation to the oxygen, giving 4--isopropoxyquinazolines, along with N^3-methylquinazolin-4-ones where the methyl group is derived from the orthoamide N-Me. The reactive intermediates are electrophilic $R^3OC(R^2)=N^+Me_2$ cations formed by thermal elimination of alkoxide from the orthoamides. This is a rare example of N- or O-alkylation by orthoamides.

The Association for International Cancer Research, Cancer Research UK, Nuffield Foundation and the University of Bath generously supported this work. HECS was a VIth form student at Bruton School for Girls during the initial part of this work.



Scheme 1. Formation of quinazolin-4-ones from anthranilamides and orthoamides and alkylation of the quinazolin-4-ones at N and O by these agents.

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Domenico Spinelli

Born in Bari (Italy) on May 30, 1932. He obtained his degree in Chemistry *magna cum laude* from the University of Bari in 1955. Assistant Professor of Organic Chemistry at Universities of Bari (1955-1961) and of Genoa (1962-1968), he was appointed to the Chair of Organic Chemistry at the Faculty of Pharmacy of the University of Sassari in 1968. After one year he moved to the Faculty of Sciences of the University of Palermo and finally (1974) to the Faculty of Pharmacy of the University of Bologna.

For a long time Coordinator of the Ph.D. Courses in Pharmaceutical Sciences and for the Degree in Pharmacy. He has been for some decades Coordinator of several National Research Projects on 'Synthesis and organic reactivity' and on 'Heterocyclic chemistry'.

Domenico Spinelli has served the chemical community for several and several years. Member of Executive Committee (1987-1992) and then President (1993-1995) of the Division of Organic Chemistry of the Italian Chemical Society; Vice-President (1996-1998), President (1999-2001), and past-President (2002-2004) of the Italian Chemical Society. He has been member of the European Committee for European Journals.

In 1974 he received the golden 'Sigillum Magnum' of the University of Palermo, and in the years he was awarded the 'A. Mangini' and the 'D. Marotta' golden medals as well as the golden 'Sigillum' of the Italian Chemical Society. Honorary life member of ISBC (India). Member of the European Academy of Sciences and Arts.

He is author of over three hundred papers (in J. Chem. Soc. Perkin Trans. 1 and 2, Chem. Commun., Tetrahedron and Tetrahedron Lett., J. Org. Chem., J. Phys. Chem. A, J. Am. Chem. Soc., J. Med. Chem., etc.) dealing with the study of the reactivity and properties of several five-membered heterocycles [thiophenes and benzothiophenes (nucleophilic aromatic substitutions); 1,2,4-oxadiazoles and isoxazoles (mononuclear rearrangements of heterocycles); imidazoles and condensed imidazoles (ring-opening-ring closing reactions); 1,3,4-oxadiazoles, 1,3,4-thiadiazoles and thiazoles (decarboxylation reactions); furans and congeners (enolisation processes); etc.]; of the micellar catalysis; of the mutagenic and antitumour properties of nitro compounds; of the pharmacological properties (LTCC blockers and agonist of MDR activity) of thiazinooxadiazolones; etc.

PL 6

ON THE DIASTEREOSELECTIVE OXIDATION OF 8-(4-BROMOPHENYL)-8-ETHOXY-5-METHYL-8H[1,4]THIAZINO[3,4-c][1,2,4]OXADIAZOL-3-ONE: A COMBINED EXPERIMENTAL AND COMPUTATIONAL INVESTIGATION

D. Spinelli

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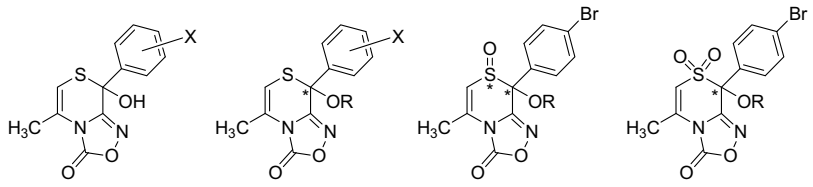
Recently we have observed that various 8-aryl-8-hydroxy-5-methyl-8*H*[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-ones (**1**)[1] and 8-alkoxy-8-aryl-5-methyl-8*H*[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-ones (**2**)[2] show an interesting activity as LTCC (L-type calcium channel) blockers. This activity is observed in some cases at nanomolar concentration. Among these species the most powerful one is 8-(4-bromophenyl)-8-ethoxy-5-methyl-8*H*[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-one (**2a**):[2b] in particular its *R*(□)-enantiomer shows a high and selective negative inotropic potency (EC_{50} 0.07 □M), which makes this compound one order of magnitude more potent than diltiazem (DTZ).

Moreover in a parallel investigation we have observed that some compounds of type **1** and **2** are promising inhibitors of MDR1 activity.[3] To obtain information on the potential activity of derivatives of sulphides **2**, eventually with the help of virtual screening procedures, we have examined the behavior of **2a** (racemic mixture: C-8 adjacent to sulfur is a chiral center) with some oxidants and we have observed that a high diastereoselectivity can characterize the oxidation process. The separation of the relevant sulphoxide **3a** (some sulphone **4a** have also been obtained) by chiral chromatography in its stereomers has allowed the assignment of the relative and absolute configuration by computational analysis of their ECD spectra.[4]



1 **2a:** R = CH_2CH_3; X = Br **3a:** R = CH_2CH_3 **4a:** R = CH_2CH_3

Furthermore, we have carried out a computational DFT investigation of the mechanism of this oxidative process.[5] The comparison between the results of 'in-laboratory-chemistry' and 'in-silico-chemistry' has provided useful information on many mechanistic aspects[6] (π-π stacking interactions and a network of hydrogen bonds) which can be essential to determine the optimum conditions favoring chemical yields of the oxidation reaction of sulphides **2** and its stereoselectivity.

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PL 7

NEW ORGANOCATALYSTS FOR THE ASYMMETRIC ALLYLATION AND REDUCTION

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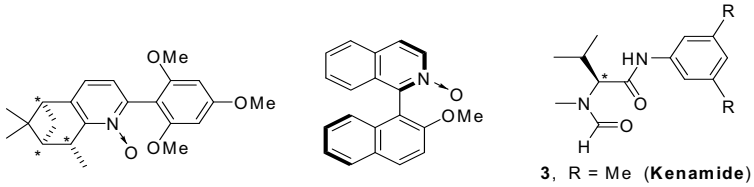
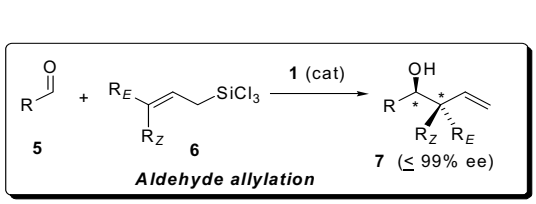
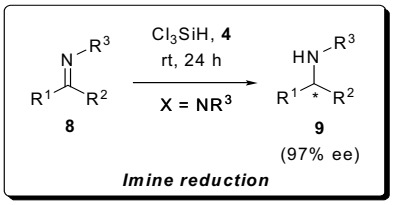
Pyridine N-monoxides **1** and **2** have been developed as organocatalysts for asymmetric allylation of aromatic, heteroaromatic, and conjugated aldehydes **5** with allyl trichlorosilanes **6** (≤99% ee, ≤99% de; at 2-5 mol% loading). Another class, the amino acid-derived formamides **3** and **4**, are efficient, metal-free catalysts for the reduction of imines with Cl_3SiH (**8** → **9**; ≤97% ee at ≥1 mol% loading).







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PL 8

CHEMISTRY AND BIOLOGY OF THE REPAIR OF OXIDIZED GUANINES

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DNA repair processes play an important role in maintaining the chemical integrity of DNA and insuring the accuracy of its informational content. The damaged base 8-oxoguanine (OG) is particularly sinister due to its subtle structural change that evades detection during replication and results in incorrect insertion of adenine to form OG:A mismatches. The MutY glycosylase prevents mutations by excising adenine from OG: A mismatches. MutY has recently been put in the spotlight based on the correlation between inherited defects in the human MutY homologue (MUTYH) and colorectal cancer,[1] referred to as MUTYH-associated polyposis (MAP). Our research laboratory provided support for the clinical correlation by analysis of the two most common variants in MUTYH revealing a hampered ability to recognize OG. We have also used a combination of synthesis of modified substrates, enzymology and X-ray crystallography to reveal features associated with damage recognition and adenine excision by MutY. Moreover, in order to correlate how defects in various aspects of the enzyme action impact repair, cellular repair assays on modified DNA substrates or with modified enzymes have been performed. Similar chemical biology approaches have been used to study the human glycosylase NEIL1 that acts upon oxidized purines and pyrimidines. Recent work has revealed that two forms of the NEIL1 glycosylase are present due to mRNA editing that have distinct differences in processing of DNA base lesions. This represents a new and unappreciated mechanism for control of DNA repair.

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Education

1994-'96 NIH postdoctoral fellowship, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA.

1989-'94 Ph.D., Chemistry, California Institute of Technology, Pasadena, CA.

1985-'88 B.S., Chemistry, Summa Cum Laude, University of North Dakota, Grand Forks, ND.

Professional Experience

Nov. '06- Professor of Chemistry, University of California, Davis

Courses: Organic Chemistry, Chemical Biology of Nucleic Acids, Physical Biochemistry, Introduction to Chemical Biology, Pharmaceutical Chemistry

Research Topics: Chemical synthesis of modified RNAs; duplex RNA binding molecules including RNA-editing adenosine deaminases (ADARs) and RNA helix-threading ligands, modulation of siRNA properties via chemical modifications

Member: UCD Chemistry Graduate Group

Member: UCD Biochemistry, Molecular, Cellular and Developmental Biology Graduate Group

Member: UCD Designated Emphasis in Biotechnology Program

2005-'06 Professor of Chemistry, University of Utah

2002-'05 Associate Professor of Chemistry (with tenure), University of Utah

1996-'02 Assistant Professor of Chemistry, University of Utah.

1994-'96 Postdoctoral Research, Harvard University.

Research Topic: Kinase activity of the mammalian target of rapamycin (mTOR)

Research Advisor: Professor Stuart L. Schreiber

1989-'94 Graduate Research, California Institute of Technology.

Research Topic: Triple helix formation with purine-rich oligonucleotides

Research Advisor: Professor Peter B. Dervan.

1992 Teaching Assistant, California Institute of Technology, Bioorganic Chemistry of Nucleic Acids.

1989-'90 Teaching Assistant, California Institute of Technology, Chemistry of Covalent Compounds I, II and III.

1988-'89 Undergraduate Research, Department of Chemistry, University of North Dakota.

Research Topic: Design and synthesis of modified nucleic acid components

Research Advisor: Professor Donald E. Bergstrom

Honors and Awards

2012	Elected as a fellow of the American Association for the Advancement of Science
2011	Selected as the alumni speaker, University of North Dakota, Dept. of Chemistry
2008-	Charter member, Synthesis and Biological Chemistry A (SBCA) Study Section, NIH
2005	Robert A. Parry Teaching Award, Dept. of Chemistry, University of Utah
2002	Camille Dreyfus Teacher-Scholar Award
1998	National Institutes of Health R29 FIRST Award (converted to R01)
1994-'96	National Institutes of Health Postdoctoral Fellowship, Harvard University.
1993	Shell Oil Predoctoral Fellowship, California Institute of Technology.
1988	Phi Beta Kappa, University of North Dakota.
1988	Dr. Walter Moran Memorial Scholarship in Chemistry, University of North Dakota.
1987	Dr. Harold W. Haugan Award in Chemistry, University of North Dakota.
1986	Dr. C.A. Wardner Memorial Scholarship in Chemistry, University of North Dakota.

Publications - 65

PL 9

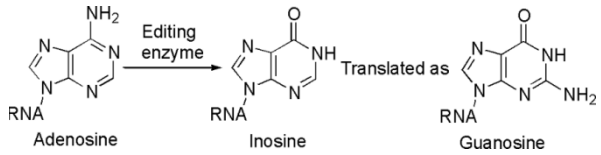
NUCLEIC ACID CHEMICAL BIOLOGY: STUDIES IN RNA INTERFERENCE AND RNA EDITING

Prof. Peter A. Beal,
Department of Chemistry, University of California, Davis, CA 95616, USA

The Beal lab is actively engaged in research at the interface of synthetic chemistry and nucleic acid biology. This lecture will cover recent studies wherein novel nucleoside analogs have been developed to explore different aspects of two RNA modification phenomena: RNA editing and RNA interference.

RNA editing. The ADAR enzymes convert adenosines to inosines in RNA in an example of base modification RNA editing. Since inosine is decoded as guanosine during translation, this modification can lead to changes in the meaning of codons (recoding). At least 50 recoding events are known in human mRNAs and perturbations in A to I editing have been observed in several human diseases. Recent efforts to define structure/activity relationships for the ADAR reaction will be described along with a newly discovered RNA editing reaction that causes recoding of the mRNA for a DNA repair enzyme.

RNA interference. Unmodified short interfering RNAs (siRNAs) are highly potent and effective at directing the selective digestion of specific messenger RNAs inside living cells grown in the lab. However, the native RNA structure has numerous drawbacks as a therapeutic agent. For instance, unmodified RNA is sensitive to nucleases, has poor delivery properties and can stimulate immune responses. While chemical modifications have been described that address these issues, the vast majority of this work has focused on structural changes to the ribose of the component nucleotides. Modification of the nucleobases can have profound effects on the chemical, physical and biological properties of oligonucleotides, yet this has been a comparatively unexplored route to the modulation of siRNA properties. Here we report the effects of newly developed base modifications for siRNAs. Purine derivatives with substituents that project into the minor groove of dsRNA are discussed that control RNAi potency, binding to off-target proteins and immune stimulation.



Vadim T. IVANOV

Born 18 September 1937. 1960 – graduated from Moscow State University. 1963 – staff member of the Institute for Chemistry of Natural Products, USSR Academy of Sciences (at present Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences) and 1988 – its Director. 1975 – Corresponding Member and 1987 – Member of the USSR Academy of Sciences (since 1992 – Russian Academy of Sciences).. 2000 – Foreign member of the Indian National Academy of Sciences. 2002 – Member of the European Academy of Sciences. 2008 Einstein Professor of the Chinese Academy of Sciences. 1980 – Professor of the Biological Department, Moscow State University. Editor-in-Chief of *Bioorganic Chemistry (*a Journal published by Russian Academy of Sciences). Scientific awards: 1975 – Lenin Prize, 1985 – State Prize, 1991 – Ovchinnikov Medal, 1997, 2005 and 2007 – Government Prizes. 2010 – Lomonosov Great Gold medal for ”Outstanding Contributions to Bioorganic Chemistry”. Author and co-author of over 400 scientific publications in various areas of peptide research:

1. Pioneering conformational studies of peptides in solution; synthesis and structure-functional studies of natural cyclic peptides; elucidation of major principles of peptide mediated transmembrane ion transport.
2. Total synthesis of snake and bee venom polypeptide neurotoxins, their chemical modification and spectroscopic study resulting in further understanding of their three-dimensional folding and the stereochemistry of interaction with membrane receptors.
3. Design and synthesis of peptides having antistress, somnogenic and immunostimulatory activity, development of respective pharmaceuticals; studies directed to totally synthetic vaccines for medical and veterinary use; identification and structure-functional studies of novel peptides from animal and plant tissues;

PL 10

PEPTIDES AS POTENTIAL BIOMARKERS FOR MEDICAL DIAGNOSTICS

V.T.Ivanov and V.M.Govorun
Shemyakin & Ovchinnikov Institute of Bioorganic Chemistry,
Russian Academy of Sciences
Moscow, Russia

Studies of potential biomarkers of human diseases in serum peptidome based on the mass-spectrometric technologies have been widely carried out in a number of laboratories in the past decade. However, these attempts have not yet produced definite results due to extreme complexity of serum composition and formidable technical difficulties, such as extensive *ex vivo* peptide formation and tight binding of peptides by huge excesses of albumin and other blood proteins. In this work we present our recent results in that area. Comparative MALDI-TOF MS profiling of blood serum samples from patients with verified ovarian cancer, colorectal cancer and syphilis as well as from a control group of healthy women has been carried out. Optimal conditions selected for sample preparation implied preliminary fractionation of serum on weak cation exchange magnetic beads followed by thermal dissociation of protein-peptide complexes. Classification models generated on the basis of respective MALDI-TOF MS profiles demonstrated sensitivity and specificity close to 100% for the detection of all studied diseases. For the identification of serum peptides the same groups of samples were sequentially fractionated using magnetic beads with weak cation exchange surfaces and strong anion exchange microcolumns. The fractions obtained were analyzed by nanoelectrospray-Q-TOF HPLC-Chip-MS/MS technique which resulted in identification of 2732amino acid sequences originating from 1778 proteins. The following analysis lead to identification of peptide families specific for concrete pathologies. Further steps to validation of the results obtained will be outlined.

In our recent experiments peptidomic approach was applied to analysis of spinal fluid samples of patients with viral and bacterial forms of meningitis. Clear differences were observed between the two forms, providing thereby ground for rapid differential diagnostics of that neurological disease. Molecular basis of the observed differences will be discussed.

Dr Sanjay Jachak

QUALIFICATION:

Dr.rer.nat. (Pharmacy)	1997	Institute of Pharmacognosy, Karl Franzens University, Graz, Austria
M. Pharm.	1994	Pune University, Pune, India

JOB PROFILE:

Year	**Designation & Place**
August 2006-	Associate Professor, National Institute of Pharmaceutical Education and Research (NIPER), Mohali, Punjab.
July 1999 – July 2006	Assistant Professor, National Institute of Pharmaceutical Education and Research (NIPER), Mohali, Punjab.
Mar 1998- June 1999	Lecturer, N.D. M.V.P. Samaj's College of Pharmacy, Nashik, Maharashtra
Mar. 1995-Feb. 1998	Austrian Research Fellow, Institute of Pharmacognosy, Karl Franzens University, Graz, Austria.
Mar. 1994-Dec. 1994	R & D Officer, Glenmark Pharmaceuticals Ltd., Nashik, Maharashtra

RESEARCH EXPERIENCE: 16 years

FIELD OF SPECIALIZATION:Natural product chemistry; isolation and characterization of bioactive compounds from medicinal plants used in inflammatory disorders, diabetes, cancer and tuberculosis; synthesis of isolated biologically active compounds, standardization of herbal drugs and formulations.

PATENTS AND PEER REVIEWED PUBLICATIONS: 64

Patents : 03 **Research Papers: 27**

Review articles: 14 **Conference presentations/abstracts: 20**

ADVISORY AND RESEARCH CONSULTANCY TO PHARMA INDUSTRY

- Vedic Life Sciences, Mumbai
- Dozo Laboratories, Mohali

GOVERNMENT RESEARCH GRANTS :

About Rs 1 crore grants from DBT, CSIR and Deptt. of AYUSH

AWARDS and HONOURS:

- Most cited paper award, Bioorganic Medicinal Chemistry Letters, 2005-2008.
- Editorial Board Member (2009-2011), Anti-Infective Agents, Bentham Science Publishers.
- Research Fellowship, Austrian Academic Exchange Service, Vienna, Austria from 1995-1998.

IL 1

DRUG DISCOVERY AND DEVELOPMENT FROM MEDICINAL PLANT-DERIVED NATURAL PRODUCTS: RECENT TRENDS AND OPPORTUNITIES FOR INDIA

Sanjay M. Jachak

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Natural products (NP) have been the most productive source of leads for the discovery and development of drugs. About 100 new products derived from NP are in clinical development particularly as anti-cancer and anti-infective agents [1]. Natural products or natural product-derived compounds represent great structural diversity which is not commonly seen in synthetic compounds. Of the 1184 new chemical entities reported during 01/1981 to 06/2006, 54% are derived from or based on natural products. Thus, natural products play a dominant role in the discovery of leads for the development of drugs for treating human diseases [2]. From India examples of three drugs viz. Flavopiridol, Forskolin, and Guggulsterone that have been discovered from natural products worth mentioning [3].

India, a country represented by rich culture, traditions, and natural biodiversity, offers a unique potential for the drug discovery researchers. In India we have two (Eastern Himalaya and Western Ghats) of the 18 worlds' hotspots of plant biodiversity and interestingly, India is 7th among the 16 countries where 70 % of the world's species occur collectively. Out of the 17,500 flowering plant species occurring in India, around 8000 are medicinal. This plant-biodiversity offers us an opportunity to undertake bio-prospecting approaches to better utilize the medicinal plants for drug discovery process [3].

NP (and traditional medicines) offers great hope in the identification of bioactive compounds and their development into drugs for the treatment of inflammatory diseases. Based on this literature survey, we have undertaken a research programme to characterize anti-inflammatory lead molecules from Indian medicinal plants that have been used in Ayurveda for treating inflammatory disorders, utilizing COX-2/COX-1 as the drug target and to design, synthesize analogues of lead molecules as potential COX-2 inhibitors. Accordingly we have studied 15 potential medicinal plant species which yielded several anti-inflammatory molecules [4-16], few of them may be considered as lead molecules for anti-inflammatory drug development. In this presentation, the attempt is being made to overview NP as an important source of drugs and to enumerate the interesting findings from our laboratory in the endeavour of drug discovery and development from herbal drugs/medicinal plants.

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Former Head and Dean of faculty of Science, Lucknow University, Lucknow, UP

Post Doctoral Visits and Position Held

1978-79: SRC, Post Doctoral Research, Robert Robinson Laboratories, University of Liverpool, UK,
1981-83: SRA, University of Groningen, Groningen, Holland
2002, 2003: Visiting Professor University of Rogensburg, Germany
1995-Till date Department of Chemistry, Lucknow University Lucknow
Jan.2008,-2010,Head of Chemistry Department, Lucknow University Lucknow
Jan.2008-2010, Dean of faculty of Science, Lucknow University Lucknow

Paper Published: > 68
Field of Interest: Heterocyclic Chemistry(Medicinal Chemistry)

IL 2

THE ROLE OF WATER IN C-N, C-S AND C-O BOND FORMING REACTIONS IN ORGANIC SYNTHESIS

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The influence of water in nucleophilic substitution reactions in organic synthesis "On-H_2O" and "In H_2O" has been demonstrated. Comparative effects of synthesis of biologically useful 1,4-quinone derivatives "On H_2O" and In H_2O" have been studied in detail.

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Dr. Arun K. Shaw

ARUN KUMAR SHAW born in July 7, 1955 did his M.Sc. in Chemistry (Organic) from University of Calcutta in 1977 and Ph. D. from University of Calcutta with Professor Subhendu N. Ganguly at Bose Institute, Calcutta in1985.

He worked as a Scientist 'B' in the Department of Food Chemistry, Central Food Technological Research Institute, Mysore-570013, India (1987-1991) and latter joined with the same capacity in Medicinal Chemistry Division, Central Drug Research Institute, Lucknow, 226001in 1991. At present he is working as a Senior Principal Scientist in Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow, India.

He has been doing research in the field of Natural Products Chemistry and Synthetic Organic Chemistry. He research group has synthesized quite a good number of bioactive natural products or natural product like molecules and anti-tubercular agents using commercially available carbohydrates as chiral pools. He is also interested in the development of new methodology/synthetic reagents and investigation of new reaction pathways in Organic Synthesis.

He has supervised seven Ph.D students and currently supervising seven students for their Ph.D degrees. He has published forty nine research papers to various journals of national and International repute.

IL 3

SYNTHESIS OF BIOLOGICALLY ACTIVE NATURAL PRODUCTS FROM CARBOHYDRATE BUILDING BLOCKS

Dr. Arun K. Shaw

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Chiron approach synthesis is a method of synthesis which utilizes the stereochemistry of the starting material. Mainly carbohydrates (monosaccharides) used as chiral pool for the synthesis of stereochemically pure target compounds. The Chiral building blocks (CBB's) derived from carbohydrates are important chiral synthons for synthesis of functionally and stereo-chemically complex natural products and natural product like molecules. Very cost effective if starting material or CBB is obtained from inexpensive sugar. Our group has reported from monosaccharides several stereochemically pure molecules that include biologically active natural products or natural product like molecules and medicinally important molecules.[1] In this conference stereoselective syntheses of few natural products by Chiron approach carried out by our group will be discussed

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Professor, Department of Chemistry
Indian Institute of Technology Madras, Chennai 600 036, India
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Education:

IIT Kanpur, India	Ph.D. (1991)	
(Prof. S. Chandrasekaran)		
Duesseldorf University, Germany	AvH Fellow (1991-93)	
(Prof. M. Braun)		
Harvard University, USA	Post-doc (1993-95)	
(Prof. E. J. Corey)		
1995 - 1998	Senior Scientist	DRF, Hyderabad
1998 – 2003	Assistant Professor	IIT Madras
2004 - 2006	Associate Professor	IIT Madras
2006 – Present	Professor	IIT Madras

Research area: Development of new strategies in Organic Synthesis; Enantioselective Synthesis; Synthesis of Biologically active Molecules & Drug Design of Pharmaceutical Importance.

Publications: More than fifty five papers in international journals and five patents in Indian and Abroad.

Honors/Awards: AvH Fellowship (Germany)
CRSI Bronze Medal
National Representative, IUPAC

IL 4

STEREOSELECTIVE SYNTHESIS OF BIOLOGICALLY ACTIVE AZACYCLIC COMPOUNDS:

Sundarababu Baskaran*

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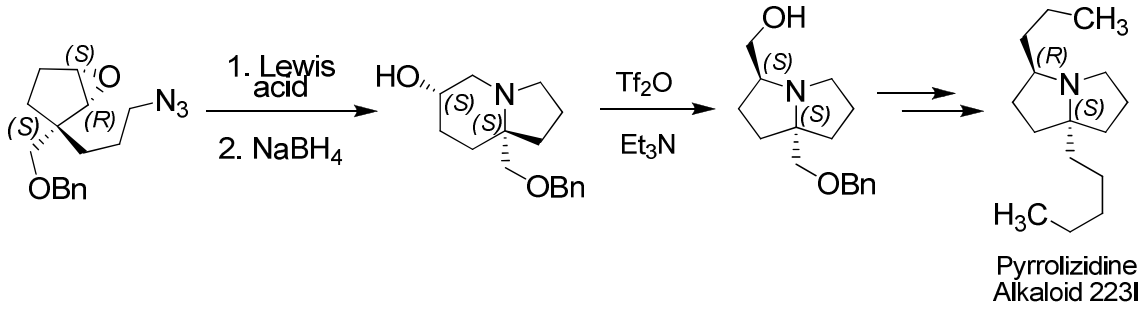
Azabicyclic ring system bearing quaternary stereocenter is a common structural feature present in many naturally occurring and biologically active molecules such as immunosuppressant FR901483, lepadiformine, polyhydroxy indolizidine and pyrrolizidine alkaloids. Alkyl substituted indolizidine and pyrrolizidine alkaloids (gephyrotoxins), isolated from skin secretion of poison dart frogs, are known to function as sodium channel activators, noncompetitive blockers of nicotinic channels and positive modulators of sodium channels. Recently, we have developed a novel and general method for the stereoselective construction of azabicyclic ring systems based on epoxide-initiated cationic cyclization of azides. This methodology has been elegantly applied in the stereo- and enantioselective total synthesis of indolizidine and pyrrolizidine alkaloids. Moreover, the stereoselective construction of azapolycyclic ring systems bearing aza-quaternary center has been developed based on *domino* semipinacol-Schmidt reaction. The application of our strategy in the stereo- and enantioselective total synthesis of pyrrolizidine alkaloid 223I will be presented.



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Diwan S Rawat did MSc from Kumaun University, Nainital in 1993 and obtained Ph.D. degree in Medicinal Chemistry from Central Drug Research Institute, Lucknow/Kumaun University, Nainital in 1998. He worked with Panchsheel Organic Limited, Indore and Lupin Laboratory Limited, Mandideep, MP and did postdoctoral work at Indiana University and Purdue University, USA. He was an Assistant Professor of Medicinal Chemistry at National Institute of Pharmaceutical Education and Research (NIPER), Mohali, before joining University of Delhi in 2003 and currently he is full Professor. Prof. Rawat has published over 55 research papers, and his work has been cited over 800 times with h-index 16. He has also co-authored a book, three book chapters, and has five patents to his credit. He has supervised seven PhD and two M Phil and currently eight students are working for PhD. His research work has been funded by Department of Science and Technology, Council of Scientific and Industrial Research and University Grant Commission. His research interests lie in the areas of development of small organic molecules as anticancer, antimalarial and antimicrobial agents. He is also working as OSD-University Press, Head, Graphic Art Center and Co-coordinator, M. Tech. (Chemical Synthesis and Process Technologies) at University of Delhi.

Prof. Rawat is a recipient of CRSI young scientist award (2007), ISCB young scientist award (2010), VC`s Pratik Chinha Samman, Kumaun University Nainital (2011) and Prof. D. P. Chakraborty 60^{th} Birth Anniversary Commemoration Award (2007), and he has delivered an invited talk at NOST 2010. He is an Associate Editor of International Journal of Drug Discovery, Journal of the Indian Chemical Society (Organic Section) and also serves on the International Editorial Advisory Board of Anti-Cancer Agents in Medicinal Chemistry, Marine Drugs, Research and Reports in Medicinal Chemistry, The Open Catalysis Journal and Chemistry and Biology Interface.

IL 5

TETRAOXANE AND AMINO-QUINOLINE SCAFFOLD BASED HYBRIDS: SYNTHESIS AND ANTIMALARIAL ACTIVITY EVALUATION

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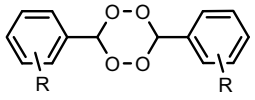
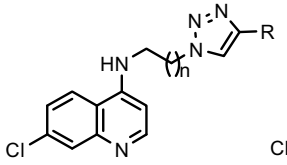
Malaria is still one of the deadly diseases causing deaths of more than 1-3 million people per year all over the world. Aminoquinolines have been used for the treatment of malaria for a long time, but *Plasmodium falciparum* has developed resistance against these compounds, and artemisinin and its derivatives are the only alternative for the treatment of *Plasmodium falciparum* related infections [1,2]. Heme and dihydrofolate reductase are the most commonly used 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 (**1**), and novel aminoquinoline-heterocycle conjugates (**2**,**3**) will be presented [7-15].



1



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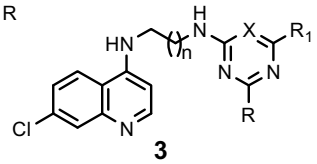

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2004-10 Assistant Professor & Head of Department, BITS, Pilani

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1997-99 Postdoctoral Fellow**,** Sam Houston State University, Huntsville, TX, USA

PUBLICATIONS:

Research Papers	: 70
Patent	: 02
Invited Lectures	: 15

IL 6

DESIGN AND SYNTHESIS OF AZAHETEROCYCLES AS NOVEL ANTITUBULIN AGENTS

Dalip Kumar

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Cancer treatment is a major challenge for the contemporary medicine. In the past, innumerable anticancer agents were developed. However, the effectiveness of most of these agents seriously suffers from the lack of tumor specificity and multidrug resistance. Microtubule plays a crucial role in the development and regulation of cell shape by involving in a range of pivotal cellular functions. Dynamic equilibrium of tubulin-microtubule is among the most successful targets to identify novel and potent anticancer agents.[1] The structurally diverse natural and synthetic analogues capable of modulating the polymerization or depolymerization of microtubules are of significant interest as chemotherapeutic agents. There are many microtubule targeting agents including taxanes, colchicine, podophyllotoxin, combreastatin, vinorelbine and vitamin K3 are known to induce cell death by affecting apoptosis. In the recent past, many bioactive indolyl heterocycles such as 3-formyl-2-phenylindoles, diarylindoles, 2-aroylindoles, arylthioindoles etc have been prepared as antitubulin agents.[2] In view of synthetic and biological importance of indole-based heterocycles and to identify potent anticancer agents, we have synthesized diverse indolyloxadiazoles, indolylthiadiazoles, bis(indoles)hydrazide-hydrazones and screened for their *in vitro* anticancer activity against various human cancer cell lines. Some of these indolyl heterocycles exhibited selective cytotoxicity against human cancer cell lines. Detailed synthesis and anticancer activity results of novel azaheterocycles will be discussed in the presentation.

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Dr. K. Avasthi

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Scientist G
Medicinal and Process Chemistry Division
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Date of birth: 24 Nov. 1952

M. Sc. Lucknow University, Lucknow 1972, Ph. D. Lucknow University, Lucknow 1976

Post-doctoral Research: 1976-1985.

1. Indian Institute of Technology, Kanpur, UP (with Prof. D. Devaprabhakara);
2. Hokkaido University, Sapporo, JAPAN (with Prof. Akira Suzuki: 2010 Nobel Prize in Chemistry);
3. University of Alberta, Edmonton, Alberta, CANADA (with Prof. E. E. Knaus);
4. University of Wisconsin, Milwaukee, Wisconsin, USA (with Prof. J. M. Cook);
5. Cornell University, Ithaca, N. Y., USA (with Prof. D. B. Collum) and
6. Case Western Reserve University, Cleveland, Ohio, USA (with Prof. R. G. Salomon).

Current Research Interest:

Molecular recognition and conformational analysis. Supramolecular Chemistry. Development of new flexible models based on pyrazolo[3,4-*d*]pyrimidine for understanding of arene (π–π) interactions. Design and Synthesis of bio-active molecules especially CNS/CVS active agents.

Publications **:** 58

Reviews **:** 02

IL 7

PYRAZOLO[3,4-d]PYRIMIDINE CORE BASED MODELS FOR STUDYING π–π INTERACTIONS IN FLEXIBLE PROPYLENE AND BUTYLIDENE LINKER COMPOUNDS AT MOLECULAR AND SUPRAMOLECULAR LEVEL

K. Avasthi,
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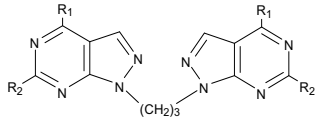
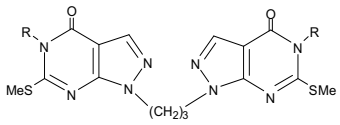
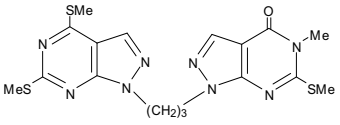
In addition to stabilization of DNA/RNA structures, arene interactions are known to play an important role in chemistry and biology particularly in molecular recognition, crystal engineering, foldamers, molecular tweezers/clips and drug development. Arene interactions studies based on **pyrazolo[3,4-*d*]pyrimidine** core, which is isomeric with purine system found in adenine and guanine two of the nucleic acid bases, in flexible *propylene* and *butylidene* linker compounds will be discussed for better understanding of π–π interactions at molecular and supramolecular level. Extensive use of X-ray crystallography and ^{1}H NMR spectroscopy for such studies to understand molecular recognition will be highlighted.



1a: $R_1 = R_2$ = SMe;
1b: $R_1 = R_2$ = SEt;
1c: $R_1 = R_2$ = S-iso-Pr;
1d: R_1 = OEt, R_2 = SMe;
1e: R_1 = O-isoPr, R_2 = SMe;
1f: R_1 = OMe, $R_2 = SO_2Me$;
1g: R_1 = OEt, $R_2 = SO_2Me$;
1h: R_1 = O-isoPr, $R_2 = SO_2Me$;
1i: R_1 = O-isoPr, $R_2 = SO_2Et$;
1j: $R_1 = R_2$ = OMe
6; R_1 = Cl, R_2 = SMe;
7; R_1 = CN, R_2 = SMe



2a: R = H; **2b**: R =Me
2c: R = Et; **2d** = CH_2Ph



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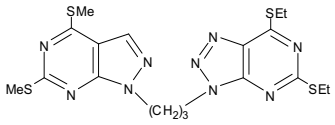

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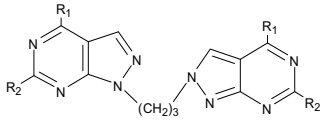

5a: $R_1 = R_2$ = SMe

Figure 1: Pyrazolo[3,4-*d*]pyrimidine core based *propylene* linker compounds.

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Qualification **:** M.Sc. Ph.D.

Area of Specialization **:** Medicinal Chemistry / Organic Chemistry

Senior General Manager : Process Development and Production (oral),.

Industrial Experience **:** About 25years of experience in pharmaceutical industry in various field like R and D, API -Process Development, Pilot Plant and Production.

Worked in Lupin Ltd for 7 years in R & D, 7 years in R & D- Orchid Pharma, and heading since11 years Process Development, Production and finished goods stores in Orchid Pharma

Articles in Journals **:** TotalNumber of Research Publications: 3

Articles communicated for publications : 03

Process Patents **:** 10

IL 8

THE ART AND SCIENCE OF CRYSTALLIZATION IN ACTIVE PHARMACEUTICAL INGREDIENT INDUSTRY (API)

Dr. R. J. Sarangdhar,

Senior G. M.: Process Development and Production (API)

Orchid Chemicals and Pharmaceuticals Ltd, Chennai.

The continuous development of the chemical process industry has been accompanied by rising demands for product quality. It is estimated that about 70% of all solid materials produced by the chemical industry by crystallization and precipitation from solution. Crystallization refers to the formation of solid crystals from a homogeneous solution. It is essentially a solid-liquid separation technique and a very important in API industry for both injectable API as well as oral API.

Crystals are grown in many shapes, which are dependent upon downstream processing or final product requirements. Crystal shapes can include cubic, tetragonal, orthorhombic, hexagonal, monoclinic, triclinic and trigonal. Different crystal shape of a same compound has different physical properties like XRD, stability, purity, bioavaibility etc.

There is need to control particle size distribution (PSD) through control of crystal growth versus nucleation and to control the purification through crystallization. The majority of pharmaceutical compounds PSD are between 5 um to 400 um and exhibit a great diversity of functional groups ranging from ionic moieties to very lipophilic or hydrophobic groups. Thus, their interactions with one another with solvents or anti-solvents and with co-solutes and impurities in solution are very diverse. The solid phases (including polymorphs and various solvates) formed by such molecules needs to be understand.

Owing to the final use of such API, strict control is required on their purity, crystal form and morphology, and particle size distribution (PSD). Control of crystallization or precipitation process is essential to obtain crystals of biochemical compounds having appropriate properties.Hence n crystallization solubility, super saturation, nucleation and growth kinetics, population balance method batch and continuous crystallizersand factors governing crystal purity, habit and morphology are relevant to the crystallization in pharmaceutical industry.

U. P. Senthilkumar

Dr. U. P. Senthilkumar completed his Master's Degree in Chemistry in 1987 in The American College (an autonomous Institution affiliated to Madurai Kamaraj University), Madurai.

Supported by CSIR Research fellowship and the prestigious Dr. K. S. Krishnan (DAE) Fellowship, he completed his Doctoral Research at the Bharathidasan University in Organic Synthesis, under the guidance of **Dr. Ramasubbu Jeyaraman**, Professor of Chemistry. His doctoral program focused on Organic Synthesis, and conformational analysis in relation to the anti-cancer properties of N-Nitroso heterocycles employing 2D NMR and several other advanced tools.

After a short period of post-doctoral research with Prof. R. Jeyaraman, he joined Torrent Research Centre, Ahmedabad, where he was involved in Process Research and Drug Discovery Research on ACE inhibitors. He focused his research on Chiral Chemistry involving Asymmetric synthesis, Chiral Prep HPLC, and stereo-selective synthesis of Active Pharmaceutical Ingredients until 1997.

In 1997, he joined Research and Development Center of Orchid Chemicals and Pharmaceuticals Ltd., Chennai. He started with the Process Research activities in non-beta lactams, and penicillins. He is currently responsible for the β-Lactams Process Research and Development**,** covering Cephalosporins, Penicillins, Monobactam, and Carbapenems. He has more than 75 articles/patents & publications, which include inventions on new products, processes, rearrangement, novel polymorphs, etc. Beta-Lactams R&D Department also focuses on New Drug Discovery on Novel Anti-infectives as well as Novel Beta-Lactam Inhibitors.

His responsibility includes Intellectual Property Management activities in the Research and Development Center, catering to the need of the Orchid Research Laboratories Ltd., Process Research Departments and Business Development Group in Orchid Chemicals and Pharmaceuticals Ltd.

IL 9

POLYMORPHISM IN PHARMACEUTICALS AND INTELLECTUAL PROPERTY

Dr. U. P. Senthilkumar,

Orchid Chemicals and Pharmaceuticals Ltd., Chennai.

Polymorphism plays a critical role in Pharmaceutical development with major impacts on the drug delivery, safety and efficacy of the medicine. Understanding of the polymorphic behaviour is as important as the discovery and development of new drug, as it can influence the whole biological behaviour of the drug substance/drug product. Inappropriate polymorph can make a drug product a toxic material and/or make it devoid of its very biological activity. In the last couple of decades the pharmaceutical industry faced several surprises at the advanced developmental stage and marketing stage with disappearing/appearing polymorphs, change in morphology, conversion of active drug into inactive drug, change in solubility, change in stability, etc., and the industry/society had to pay heavy price for its ignorance. Hence, continued efforts have been put by pharmaceutical R&D centres to identify the appropriate polymorph in the early stage of drug development in order to exercise control of the pharmacological properties throughout the life time of the drug product form R&D to its delivery in patients throughout the process of manufacturing, formulation, packaging, storage in pharmacies, and dispensing. In parallel with the research on polymorphism, lot of analytical techniques/equipment have been developed to identify and study the polymorphs and their behaviour. Needless to say that the complex polymorphic behaviour of drug substances/drug products and the polymorphic screening led to the generation of intellectual property, and subsequent patenting by all the pharmaceutical research and development centres. It has also become a topic of discussion of life cycle extension by the pharmaceutical companies. The discussion will talk about various dimensions of polymorphism, the opportunities and the risks of new polymorphs, and the associated Intellectual Property.

Dr. Balasubramanian Gopalan

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Doctorate Degree (1976) in Synthetic Organic Chemistry, University of Madras.

HARVARD University, USA (1977-79): Worked with Professor E.J.Corey (Nobel Laureate in Chemistry) on the Total Synthesis of Gibberellic acid.

Syntex Research Inc., California, USA: International Post-Doctoral Fellow (1979-80). Synthesis of unnatural amino acids using Chiral transformation reagents.

Bristol-Myers Squibb, Princeton,Newjersey,USA: Research Associate in the Division of Organic Chemistry (1980-82). Engaged in the design and development of Monobactam Antibiotics and ACE inhibitors.

Boots Pharmaceuticals (India) Ltd(1982-92), Drug Discovery Research Division.

Drug design and development of oral antidiabetic agents, oral ant-amoebic agents and anti inflammatory agents(inhibition of Monocyte chemotaxis).

Sun Pharma Advanced Research Centre, Baroda. Vice President (1992-93), R&D (Organic Synthesis). Engaged in Process Development Research on Pharmaceuticals.

Glaxo (India) Ltd, Mumbai (1993-1999). Sr. Vice President, R&D. Process R&D & Drug Discovery (Glaxo- France in the Cardiovascular Therapeutic segment)

Glenmark Research Centre(Dec 1999-2005,Mumbai). Involved in the Design & Development of PDE IV Inhibitors (Asthma, COPD, RA & MS), DPP IV inhibitors (Type 2 Diabetes) and CB2 Agonist (NeuropathIc Pain).

Matrix Laboratories Ltd(2005-2008) CSO & Executive Vice President (Drug Discovery Research). Developed Leads MX-4007 (a novel PDE4 Inhibitor). MX-6001 (a novel selective,DPP4inhibitor).

Orchid Chemicals & Pharmaceuticals Ltd: Chief Scientific Officer and Executive Director.

Drug Design & Development in the Therapeutic segments of Oncology, Anti-invectives, Anti-inflammatory & Metabolic Disorders.

Some of the Achievements:

1. Diabetic candidate, **BTS-67582 (BTI2927**) went up to Phase-2 Clinical Trials in USA & UK. as an oral anti-diabetic agent.
2. **Oglemilast** (GRC3886, a novel PDE IV inhibitor) was out-licensed to Forest Laboratories, USA, for US$190 million over a period of Five years & also to Teijin of Japan for US$53 million.
3. **Melogliptin** (GRC-8200,a new DPP4 inhibitor for Type2 Diabetes) was out-licensed to Merck KGaA, Germany for US$231 million.

Artcles and Patents : Twenty three (23) publications in International Journals. Sixty four (64) International Patents

IL 10

GREEN CHEMISTRY: BASIC PRINCIPLES & ATOM ECONOMY

B.Gopalan, Ph.D,

CSO, Orchid Research Laboratories Ltd

Green chemistry is an inventive science based on fundamental research towards the development of new sustainable chemical processes.Green chemistry is defined as the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design,manufacture and application of chemical products.

The principles of Green chemistry provide a framework for a rational design of environmentally friendly chemicals and chemical processes having reduced intrinsic hazard.It is important for our Academic community to make advances in key areas,developing new catalysts,solvents,polymers,plastics additives and biomass transformations that add to the 'Tool box' of alternative,more benign & transformative technologies.It is a new partnership,bringing together the efforts of Industrial and Academic research and building rapidly on the past successes of both.

Implementing the Twelve green chemical principles requires a certain investment,since the current,very expensive chemical processes must be redesigned.However,in times when certain raw materials become more expensive and also the costs of energy increase,such an investment should pay back as the optimized processes become less expensive than the unoptimized ones.The development of greener procedures can therefore be seen as an investment for the future.

Green chemistry for chemical synthesis addresses future challenges in working with chemical processes & products by inventing novel reactions that can maximize the desired products and minimize by-products,designing new synthetic schemes & apparati that can simplify operations in chemical productions & seeking greener solvents that are inherently environmentally & ecologically benign.

Besides the basic principles[1] of green chemistry in general,a special reference to atom economy[2]& its applications to pharmaceuticals & fine chemicals would be discussed in detail.

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8. J Org Chem76,p4379-91 (2011)
9. Pure & Applied Chem 83(7),p1379-90 (2011)

Ashok K Prasad
Professor, Department of Chemistry, University of Delhi
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, INBRE Lecture Award, College of Pharmacy, Rhode Island, USA and Visiting Associate Professorship, Department of Physics and Chemistry, University of Southern Denmark, Denmark (July 2009-June 2010)

Has been the Guest editor for many International Journals including *Biochemie*, a journal published by Elsevier (Impact Factor ~4)

Publications	: 150 Research Papers in the International Journal of Repute
Total Citations of his Publications	: 1550
***h* Index** of his publications	: 20
Patents	: 10 International and Indian Patents in his credit

IL 11

BACKBONE MODIFIED NUCLEIC ACIDS AND SUGAR-PEG BASED POLYMERIC ARCHITECTURE OF IMPORTANCE

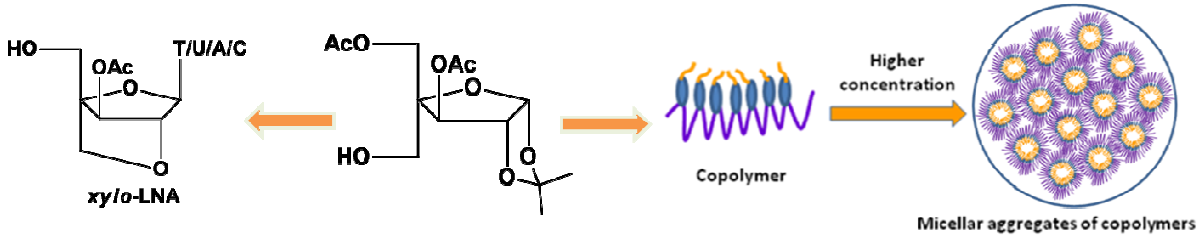
Ashok K. Prasad

Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi-110 007

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.



Acknowledgements: We thank the University of Delhi (DU-DST Purse Grant) and the International Division, Department of Biotechnology (DBT, New Delhi) for financial assistance.

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Dr. Nitin T. Patil

Nitin T. Patil was born in Jalgaon (Maharashtra), India, in 1975. He completed his doctoral study at University of Pune in 2002 under the supervision of Prof. D. D. Dhavale. After working as a post-doc at Goettingen with Professor Christoph Schneider, he moved to Tohoku University, Japan, as a JSPS fellow. Later, in April 2005, he was appointed as Assistant Professor in Prof. Yoshinori Yamamoto's laboratory. In June 2006, he joined Prof. K. C. Nicolaou's laboratory (PI: Prof. David Chen) at Singapore, and later at The Scripps Research Institute, USA.

He began his independent career in September 2008 at IICT, Hyderabad, India. He has been the recipient of INSA Young Scientist Medal - 2010 and Alkyl Amines – ICT Foundation Day Young Scientist Award – 2010. He has also been elected as "Young Associate" of the Indian Academy of Sciences, Bangalore in 2010. His broad research interests include development of metal-, organo- and metaloorgano-catalyzed enantioselective methods and total synthesis of natural products.

IL 13

BRANCHING CASCADES IN DIVERSITY ORIENTED SYNTHESIS

Dr. Nitin T. Patil
Senior Scientist, Organic Chemistry Division - II
Indian Institute of Chemical Technology; Hyderabad - 500 607
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A key challenge in chemical biology or drug discovery is the identification of new modulators of biological systems. Traditionally new lead compounds have come from nature or from combinatorial chemistry. Diversity-Oriented-Synthesis (DOS) also aims to meet this challenge by creating complexity from simple starting materials to generate libraries of diverse complex molecules. Several strategies for DOS have emerged since Schreiber coined the term in the late 1990's [1]. Recently, the "branching pathway" strategy has been proposed as a form of DOS[1]. In this strategy, a common substrate is transformed into structurally diverse molecular scaffolds.

Our efforts in the development of novel catalytic branching cascade will be briefed in this presentation (Fig 1)[1]. The presentation will also highlight the possibility of developing catalytic enantioselective variants under a co-operative catalysis of metal complexes and chiral organocatalysts[2].

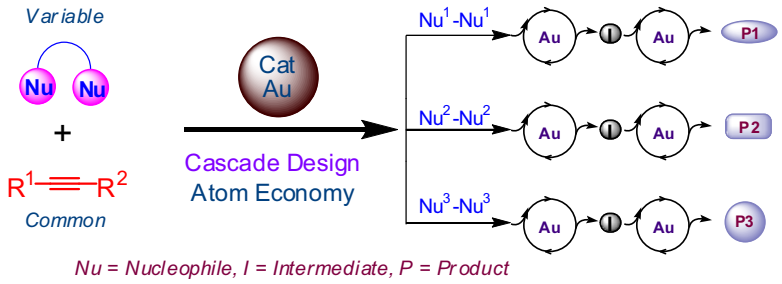

Figure 1. Novel Branching Cascades

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Dr. P. T. Perumal
Chief Scientist and Head
Organic Chemistry Division
Central Leather Research Institute
Adyar, Chennai – 600 020

ACADEMIC RECORD

- M.Sc.(Organic Chemistry) First Class Madurai University 1976
- Ph.D (Organic Chemistry), I.I. Sc., Bangalore 1981
- D. Sc.,(Organic Chemistry), University of Madras, Chennai 2010
- Postdoc Purdue University (1981-1983), University of Miami (1989-1990), University of Florida (1990- 1991).
- Visiting Professor University of Complutence, Madrid (2005 and 2008) and University of Oklakoma, (2007)
- Guided 30 Ph.D students
- Paper published 290 in peer reviewed journal
- Teaching experience 28 years
- Currentl guiding 10 students

AREAS OF SPECIALIZATION

- Synthesis of heterocyclic compounds by using Vilsmeier reagent, Diels-Alder reaction, multi-component reactions and green chemistry methodologies.

HONOURS AND AWARDS

2. Tamil Nadu State Council for Science and Technology Award for Chemistry (2002)
3. Chemical Research Society of India (CRSI) Bronze medal (2005)
4. Best Paper award- INDO-US Conference, held at IIT, Chennai, India (2003)
5. Prof. S. Swaminathan endowment lecture award 2009
6. Tetrahedron- Most cited Paper award 2005-2008
7. Tetrahedron Letter- Most cited Paper award 2006-2009
8. Best thesis award for my student Dr. G. Savitha 2009.
9. Fellow of Tamil Nadu Academy of Science 2010
10. Best thesis award for my student Dr. C. Praveen 2011.

IL 14

CARBOCYCLIC AND HETEROCYCLIC COMPOUNDS SYNTHESIS FROM ALKYNES AND NITRILES

Dr. P.T.Perumal,
Chief Scientist & Head
Organic Chemistry Division, Central Leather Research Institute, Chennai-600 020.

Carbon-carbon bond formation is probably the most useful transformation in synthetic chemistry. Transition-metal-mediated C-C bond-forming reactions involving alkynes have been extensively investigated on the basis of the fact that they produce a variety of interesting organic compounds, such as conjugated olefins, unsaturated cyclic hydrocarbons, α,β-unsaturated aldehydes, unsaturated cyclic ketones, enynes, alkyne polymers, arenes, heteroarenes, and others. Alkynes react with transition metals to yield stable complexes in several ways: (i) reactions of internal alkynes mostly yield π- alkyne complexes ; (ii) those of terminal alkynes frequently yield alkynyl complexes; (iii) metallacyclopentadienes are obtained from the reactions of internal and terminal alkynes, depending on the metals and the alkyne substituents; and (iv) alkynes are inserted into the M-L bonds to produce alkenyl complexes. π-Acidic transition metal-catalyzed intramolecular addition of a heteroatom to an alkyne and subsequent migration of the substituent is one of the most powerful strategies for the synthesis of heterocyclic compounds. These transformations have provided useful access to benzofurans, indoles, benzothiophenes, furans, pyrans, pyrrolidine, and isoxazoles.

Currently our research group mainly focusing in the synthesis of heterocycles such as quinolines, furans, chromenes, isoxazoles, triazoles *via* intermolecular dimerization of 2-ethynyl anilines, sequential cycloisomerization/C3-functionalization of 2-ethynylanilines, furannulation of 2 alkynylcycloalk-2-enols, cycloisomerization of 2-alkyn-1-one (*Z*)-oximes using gold catalyst. Some interesting spirocyclic oxindoles, indolyl pyridines are also synthesised using isatylidene malononitriles, 3-cyanoacetyl indole as starting materials involving the intamolecular nucleophilic addition of heteroatom to the nitrile group. Conversion of alkynes and nitrile to cyclic compounds will be discussed in detail.

NARSHINHA P. ARGADE, Ph.D.

Scientist

Division of Organic Chemistry

National Chemical Laboratory (CSIR)

Pune 411 008, India

np.argade@ncl.res.in, npargade@yahoo.com

- Twenty seven years research experience in basic and applied organic chemistry with 89 publications in national and international journals.
- Areas of Organic Synthesis - Heterocycles, Steroids, Pheromones, Bioactive Natural Products, Drugs, Drug Intermediates, Asymmetric Synthesis, Biotransformations and Combinatorial Chemistry.
- Creativity - Development of novel chiral and achiral synthetic routes and processes.
- Recognized as a Research Guide in Chemistry for Pune University.
- Training with eminent chemists - Dr. V. Balasubramaniyan (Doctoral work, 1984-89), Dr. S. Rajappa (RA, 1990-92) and Prof. Kenji Mori (Post-doctoral work, 1993-94) with national and international scholarships.
- Senior scientist at NCL, Pune since 1994.
- Delivered several lectures in India, Japan, Italy, China, Thailand and France.
- Eleven students have got Ph. D. Degree and supervising Ph. D. dissertations work of eight research scholars.
- Successfully completed several Industry and DST-sponsored projects.
- Prof. V. V. Kogekar First Rank Award 1984.
- Fellow of Maharashtra Academy of Sciences.
- The Chemical Research Society of India Young Scientist Award 2002.
- Indian Science Congress Association, Professor R. C. Shah Memorial Lecture Award 2002-2003.
- Visiting Associate Professor at The University of Tokyo, Tokyo, Japan (June 2004-November 2004).
- Organized ICS-UNIDO-NCL-Workshop on combinatorial chemistry and biodiversity at NCL, Pune (December 2006).
- Professor N. S. Narasimhan Trust Endowment Prize for Research in Chemistry - 2006.
- Regular reviewer for Journal of Organic Chemistry and Organic Letters

IL 15

REMARKABLY SELECTIVE NUCLEOPHILIC REACTIONS OF CYCLIC ANHYDRIDES AND DERIVATIVES: SYNTHESIS OF NITROGEN CONTAINING BIOACTIVE NATURAL PRODUCTS

Narshinha P. Argade

Division of Organic Chemistry, National Chemical Laboratory (CSIR), Pune 411 008, India

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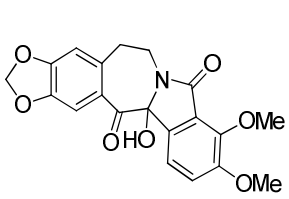
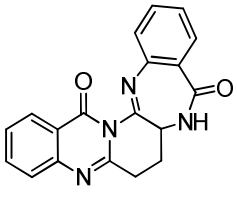
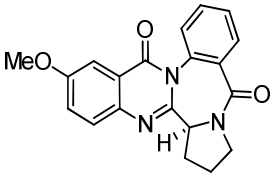
The cyclic anhydride is an important functionality in synthetic organic chemistry and the starting material of choice for all chemists from both the basic and applied point of view for multipurpose. We reasoned that with proper control on reactivity and selectivity, the cyclic anhydrides would be the potential starting materials for the synthesis of bioactive natural products. We have performed remarkable chemo-, regio- and stereoselective nucleophilic reactions on cyclic anhydrides and their derivatives with the carbon, nitrogen, oxygen and sulfur nucleophiles to accomplish the total synthesis of several bioactive natural products in a concise and efficient manner employing variety of new synthetic strategies. A concise account on synthesis of several nitrogen containing bioactive natural products will be presented with a special emphasis on the involved decisive steps.[1-5]



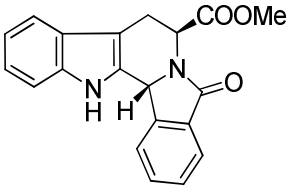
Chilenine



Auranthine



(-)-Circumdatin H



(+)-Isoindolecarboline

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Dr. D. Srinivasa Reddy Scientist

Organic Chemistry Division

National Chemical Laboratory Pune 411 008.

ds.reddy@ncl.res.in

Research Interests: Synthesis of biologically active compounds, Medicinal and Bioorganic chemistry

11/2010-present	**Scientist**, Division of Organic Chemistry, National Chemical Laboratory, Pune,
04/2010-10/2010	**Section Head**, Discovery Chemistry, Advinus Therapeutics Pvt. Ltd, Pune, India.
11/2007-03/2010	**Group Leader**, Discovery Chemistry, Advinus Therapeutics Pvt. Ltd, Pune, India.
01/2007-10/2007	**Research Investigator**, Discovery Chemistry, Dr. Reddy's Laboratories Ltd., Hyderabad, India.
12/2003-12/2006	**Principal Scientist**, Discovery Chemistry, Dr. Reddy's Laboratories Ltd., Hyderabad, India.

Pharma career 2004-2010 (Dr. Reddy's & Advinus):

- Worked in drug discovery for seven years. During this period, gained experience in leading various drug discovery programs, particularly, in the area of metabolic disorders.
- Acquired skills in designing novel small molecules and optimization for improving potency and drug like properties.
- Two projects at Dr. Reddy's and Advinus went through full cycle of hit identification, hits-to-leads and lead optimization phases and led to optimized drug candidates. ***One of the molecule is in phase-I human clinical trials where I was a project leader.***
- The work from both Dr.Reddy's and Advinus resulted in several patents (9-filed and 8-published)
- While working in industry, executed some of independent research ideas with the help of team members and published in peer reviewed journals (about a dozen publications).

Academic:

- **Post-doctoral 2000-2003 (*Prof. Sergey A. Kozmin - University of Chicago & Prof. Jeffrey Aubé - University of Kansas*):** (i) Developed new synthetic methodologies applied them to synthesis of biologically active natural products. (ii) Synthesized cyclic peptides (□-turn mimetics) for deamidation studies. (iii) Designed and developed chemistry on solid–phase for the synthesis of functionalized Freidinger-lactams and □-turn mimetics.
- **Ph.D. 1996-2000 (Prof. Goverdhan Mehta - University of Hyderabad/IISc):** (i) Trained in basic organic synthesis (ii) Acquired skills in planning and execution of total synthesis of biologically active natural and unnatural products.

IL 16

PANTOLACTONE CHIRAL POOL APPROACH: SYNTHESIS OF BIO-ACTIVE NATURAL PRODUCTS

D. Srinivasa Reddy

CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune, 411008, India.

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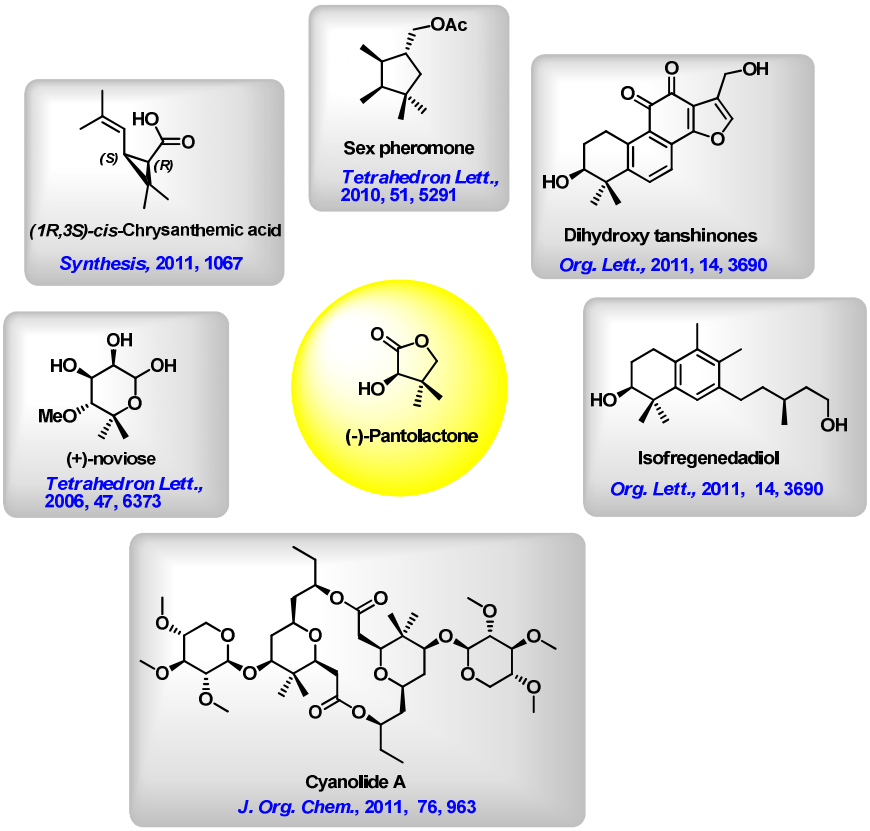
In my presentation, I will talk about our group efforts on synthesis of various natural products of biological interest using abundantly available chiral pool (-)-pantolactone as a starting material. Focus will be on recent on results.



Datta E. Ponde

Office address	: Director Deccan Institute of Chemical Technology Shriram towers, Opposite Jogging Park, Professor colony Savedi, Ahmednagar 414 001
Visiting Scientist	: University of Pennsylvania; 420 Curie Blvd, Cyclotron Facility Philadelphia, PA 19104; USA
Citizenship	: Indian (Permanent Resident or Green card holder of USA)
Education	: 1998 Ph. D.; (Synthetic Chemistry), NCL, Pune University Pune, India
Ph. D Thesis title	: Total Synthesis of Camptothecin, Resorthiomycin and Applications of Heterogeneous Catalysts in Organic Transformations
Industrial experience chemist	: Lupine Laboratories Ltd, Bhopal; Aug 1990 to June 1992, R& D
Post-doctoral Appointments	: May 1999- Jan 2001: The Hebrew University of Jerusalem, Israel with Professor Raphael Mechoulam.
Research Associates	: Feb 2001-Dec 2004: Washington University in St. Louis with Professor Michael J. Welch
Faculty Appointments	: Jan 2005- March 2011 Assistant Professor; Department of Radiology; University of Pennsylvania, Philadelphia, USA
March 2011-	Present Director; Deccan Institute of Chemical Technology, Ahmednagar, India

Membership in Professional and Scientific Societies:

2001- American Chemical Society
2002- Indo-US Society of Nuclear Medicine
2001- Society of Nuclear Medicine
2004- Society of Radiopharmaceutical Sciences

Honors and awards:
Pilot research award from Society of Nuclear Medicine, USA, 2006
Seed research award from Abramson Cancer Center 2006-07
Prof. B. D. Tilak Visiting Fellowship 2008-09 from University of Mumbai, India
"New Investigator Award" from US Department of Defense 2009-11

Total Publications 34 and Total Citations 560

IL 17

ROLE OF BIOMEDICAL IMAGING IN MODERN DRUG DISCOVERY

Dr. Datta E. Ponde
Director
Deccan Institute of Chemical Technology, Ahmednagar 414 001

New drug discovery is very risky, lengthy and complicated research and development area. Out of various approaches, biomedical imaging has been evolved as a promising multidisciplinary area which has ability to give valuable inputs for drug discovery. Understanding pharmacokinetics (PK) and pharmacodynamics (PD) profiles are key to translation of New Chemical Entity (NCE) from pre-clinical to clinical stage. Radiolabeling of NCE by short lived isotopes and following their path and accumulation in body can be very useful for PD/PD studies and will make drug discovery affordable and will reduce time between pre-clinical to clinical translation.

Dr. M.M.V.Ramana

DESIGNATION : Professor of Organic Chemistry
ADDRESS : University Department of Chemistry, University of Mumbai
EMAIL : mmvramana@chem.mu.ac.in; mmvramana@yahoo.co.in
MOBILE No. : 08767032849

TEACHING EXPERIENCE : 26 Years

RESEARCH GUIDANCE :

Degree	Degree awarded	Working at present
Ph.D.	15	10
M.Sc. (By Research)	16	Nil

RESOURCE MOBILISATION : DST Project (Rs. 10 lakhs)
PUBLICATIONS : 30
PATENTS : 17
BOOKS : 01
AREAS OF RESEARCH :

1. Synthesis of Natural Products.
2. Identification and Resolution of Conglomerates.
3. Use of Non – Conventional Sources of Energy.
4. Green Chemistry.
5. Design and Synthesis of New Drug Entities..
6. Synthesis of Soft Materials for Nanotechnology.
7. Synthesis of Macromolecules.
8 Synthesis and characterization of New and Novel Liquid Crystalline Materials

IL 18

Domino Reactions

Prof. M. M. V. Ramana,

Professor of Organic Chemistry,

University of Mumbai.

The presentation describes a brief review of Domino Reactions and its application for the synthesis of natural products like, Alkaloids, Terpenoids, and Fluorenones carried out in our laboratory. Many of these natural products exhibit wide spectrum of biological activities.

Prof.B.Kesava Rao, M.Sc., Ph.D
Former Chairman-Board of Studies &
Head of the Department of Chemistry
Acharya Nagarya University
Nagarjuna nagar-522 510

Prof.Bhattiprolu Kesava rao was born at Challapalli, Krishna District, Andhra Pradesh on 10th July 1958 to his beloved parents Sri.Bh.V.Ramana Rao and Smt.B.Subbalakshmi. His father belongs to the first batch of students of Andhra University and completed his service as a Senior Science teacher at SRY. Siva Rama Krishna Prasad Bahaddur High School & Jr.College at Challapalli. Dr.B.Kesava Rao had his basic education in the same school and later joined in Andhra Loyola College for his Intermediate & B.Sc Degree with Chemistry (Main) and Physics & chemistry as ancillaries. Later, he has selected Nagarjuna University for his M.Sc., Degree with Organic Chemistry as Specialization during (1977-79). By the Grace of His beloved God, he got a chance to join as a research Scholar under the guidance of Prof.K.V.Jagannadha Rao, Chairman & Head, Dept.of Chemistry in January 1980 and got his Ph.D degree with the Title: **"Novel Quinones from the root bark of *Ventilago calyculata*** Tul. (Rhamnaceae) in 1984 from Nagarjuna University.

As a Post Doctoral Research Fellow in the University of Kansas, Lawrence, USA, Dr.Kesava Rao actively participated in a special project on " **Investigations into Antibiotics, Anticancer and Antimutagenic Agents"** supported by National Institute of Health **(NIH) ,USA** under the guidance of the **Distinguished Professor Lester A. Mitscher, Medicinal Chemistry, School of Pharmacy, University of Kansas, Lawrence, U.S.A.** During that period he had the opportunity to screen the plant ***Krameria triandra*** (Krameraceae) and the **Lichen *Alectoria sarmentosa*** and found to be active against Gram positive , acid-fast and fungal microorganisms. The activity and structural elucidations of these compounds were also established. There he was also specialized in the isolation of most difficult and clinically needed anticancer agent **Taxol** from ***Taxus brevifolia*** **(Taxaceae).**

When Dr.B.Kesava Rao was in India as a Research Associate-UGC and had the collaborative research work with **Professor Noboru Motohahi**, **Meiji College of Pharmacy, Tokyo, Japan** on **"Synthesis and Activity of Antitumor Ferrocenes and Phenothiazines."**

In the earlier investigations certain Medicinal plants belonging to the botanical family Rhamnaceae were examined and about **fifteen new Quinones** were isolated and had the active collaboration with Professor Ronald.H.Thomson, University of Aberdeen, Scotland, U.K. Synthesis and Pharmacological studies of some of these compounds were also in progress. During his entire carrier he has established active collaboration with Pharmaceutical Industries and Overseas laboratories from USA, UK, JAPAN, CHINA, FRANCE, SOUTH AFRICA, HUNGARY and recently with KOREA. He has published more than 20 papers in reputed International Journals.

IL 19

HEALTH AND WELLNESS-NATURALLY OCCURRING PENTACYCLIC TRITERPENES FROM THE GENUS CALOTROPIS (FAM: ASCLEPIADACEAE)- A REVIEW

Bhattiprolu Kesava Rao*, Saketi Jagan Mohan Rao, Vustelamuri Padmavathi

and Noboru Motohashi**

*Prof.B.Kesava Rao, Head Dept.of Chemistry, University College of Sciences, Acharya Nagarjuna University, Nagarjunanagar-522 510, Guntur District, Andhra Pradesh, India. krbhattiprolu@gmail.com**Prof.Noboru Motohashi, Meiji Pharmaceutical University, 2-522-1, Noshio, Kiyose-shi, 204-8588, Tokyo, Japan. noborumotohashi@jcom.home.ne.jp

The triterpenes are the compounds which constitute a larger diverse group of natural products with a carbon skeleton based on six isoprene units, and which are derived biosynthetically from the acyclic C_{30} hydrocarbon, sqalene or in the case of 3β-hydroxy triterpenoids, the 3S-isomer of sqalene 2, 3-epoxide. These were colorless, crystalline, often high melting, and optically active substances, which are generally difficult to characterize because of their lack of chemical reactivity. Biologically these are extremely active and some of them are even poisonous. Pentacyclic triterpenoids were occurred especially in the waxy coatings of leaves and fruits, and they may serve a protective function in repelling insect and microbial attack. These were also found in resins, barks of trees and in latex. Certain triterpenes were notable for their taste properties particularly their bitterness. These were comprised of various sub groups, eg.Oleanane group (β-amyrin), ursane group (α-amyrin), taraxastane group (taraxasterol) and Lupane group (Lupeol). Formation of a six-membered ring E from bacchrane precursor leads to the oleanane group. Oleananes from the largest group of triterpenoids and occur widely in the plank kingdom often as glycosides. Methyl migration in ring E of the oleanane precursor leads to the taraxastane skeleton or to the stereo isomeric ursane skeleton. In general, formation of a five membered ring E from the bacchrane precursor affords the lupine skeleton.

The above groups pentacyclic triterpenes are the main constituents of the root-bark of *Calotropis gigantea* and *C.procera*, and also present in various parts of the plant. In our study we found the presence of these compounds in root-bark leads to very important role in clinical therapy, i.e., the root-bark of C.gigantea and C. procera, is useful in curing skin diseases, enlargement of abdominal viscera, intestinal worms, cough, ascites, anasarca, snake-bite, tooth-ache, dysentery and Syphilis. More than 30 naturally occurring pentacyclic triterpenes were reported from the *Calotropis* till today. The physical parameters of the naturally occurring pentacyclic triterpenes obtained from *Calotropis* were given in this paper as a special review followed by the structural elucidation, confirmed by their spectral evidence from UV,IR, ^{1}H & ^{13}C NMR and their characteristic mass fragmentation studies will be clearly discussed. The medicinal properties of the active compounds of this special category will also be mentioned.

IL 20

SYNTHESIS OF SOME NOVEL INDOLE DERIVATIVES USING DEXOYBENZOINS AS INTERMEDIATES

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Indoles exhibit anticancer, antiviral, antibacterial, antioxidant, cytotoxic and insecticidal activities. The indole moiety is present in a number of drugs currently present in the market. Most of these belong to "triptans" which are used mainly in the treatment of migraine headaches. All members of this group are agonists of migraine associated 5-HT_{1B} and 5-HT_{1D} serotonin receptors [1]. Sumatriptan (Imitrex) was developed by Glaxo for the treatment of migraines and introduced into the market as the first member of the triptan family [2].

The indoles **(4BPP001)** were synthesized from dexoybenzoins and substituted aryl hydrazines [3,4]. The compound **4BPP001** was reacted with methyl iodide under K_2CO_3/DMF condition and NH_4Cl under Py-BOP/HOBT/TEA to give alkylated **(4BPP002)** and amide **(4BPP003)** derivatives respectively. Aryl boronic acids were treated under Suzuki condition (Pd_2dba_3, X-phos, Na_2CO_3, ACN: H_2O) in microwave to afford various Suzuki coupled products **4BPP004-4BPP024**. Finally, free acid group of **4BPP001** reacted with different amines in presence of EDC.HCl, HOBT in basic medium to afford acid amine coupled products **4BPP025-4BPP029**.

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Research Fellow,
Griffith University, Brisbane, Australia.
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Academic Qualification

Aug 2003-May 2007: Ph.D. Chemistry, Indian Institute of Chemical Technology, Hyderabad, India.

June 1998-June 2000: M.Sc. Chemistry (Drugs & Pharmaceuticals), Swami Ramanand Teerth Marathwada University, Nanded, India.

Academic Awards & Fellowships

- 2003 - Awarded ***Junior& Senior Research Fellowship*** (UGC-CSIR based on national aptitude screening test conducted by Govt. of India).
- 2002 - Qualified **NET** (National Eligibility Test for Lectureship conducted jointly by CSIR-UGC) examination.
- 2002 - Qualified **MHSET** (Maharashtra State Eligibility Test for Lectureship conducted by University of Pune, accredited by UGC) examination.
- 2002 - Awarded **G. D. Gokhale Fellowship** for Ph.D. at University Institute of Chemical Technology (Formerly UDCT), Mumbai.

Research Training

Post Doctoral Research

May 2009-Present: 'Natural product based drug discovery against Tropical diseases' *Advisor*: **Prof. Ronald J. Quinn**; Director - Eskitis Institute for Cell and Molecular Therapies, Griffith University, Brisbane, Australia.

May 2007-Feb 2009: 'Marine natural product synthesis and drug discovery against metabolic diseases like obesity, type II diabetes' *Advisor*: **Prof. Heonjoong Kang**; Director - Center for Marine Natural Products & Drug Discovery, Seoul National University, Seoul, South Korea.

Doctoral Research

Aug 2003- May 2007: 'Isolation and structure elucidation of novel anticancer agents and synthesis of small bioactive molecules using new synthetic methods' *Advisor*: **Dr. Biswanath Das** (**FRS**); Deputy Director - Indian Institute of Chemical Technology, Hyderabad, India.

Publications: 27 articles in International & National Journals.

Invited talks & Posters at International conferences: 2 & 4

IL 21

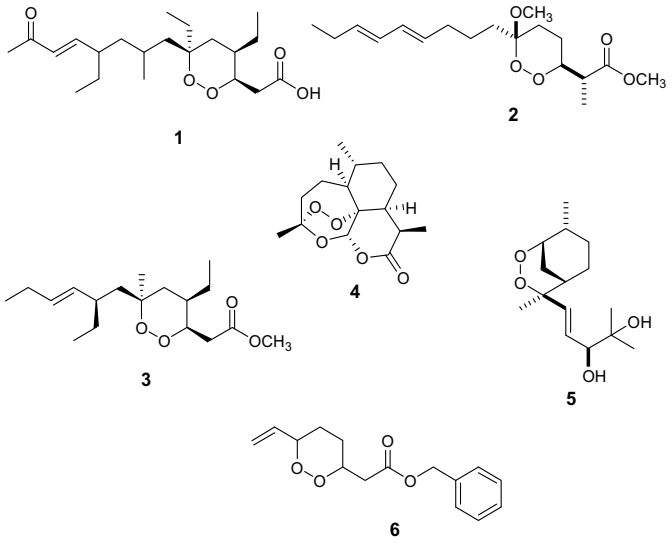
NATURAL PRODUCT SCAFFOLD BASED LEAD OPTIMIZATION AGAINST TROPICAL NEGLECTED DISEASES

Harish Holla, Ronald J. Quinn*
Eskitis Institute, Griffith University, Brisbane, QLD-4111, Australia.

Human African Trypanosomiasis (HAT) and Malaria are two of the world's deadliest diseases, with more than one million deaths worldwide in 2008, most of them in sub-Saharan Africa and Asia. Owing to the complexity of these diseases and to the emergence of parasites that are resistant to currently available anti-HAT and antimalarial drugs, there is an urgent need for effective and affordable drugs.

Several cyclic peroxides isolated from marine sponge *Plakortis* species such as 11,12-didehydro-13-oxo-plakortide Q (**1**) exhibited antitrypanosomal activity at an IC_{50} 49 nM against *Trypanosoma brucei brucei*. While peroxyplakortic acid B_3 (**2**) and plakortin (**3**), along with a number of analogues from *Plakortis simplex,* have shown sub-micromolar *in vitro* antimalarial activity. A comparison of **1**-**3** with the known antimalarial artemisnin (**4**) and yingzhaosu A (**5**) suggested that the substituted 1,2-dioxane moiety might be the core skeleton responsible for the antimalarial and antitrypanosomal activity.

A short practical synthesis of a new natural product inspired scaffold (**6**) is carried out. The scaffold contains a peroxide unit that is surprisingly stable to chemical manipulations like ozonolysis, reductive work-up with dimethyl sulfide and the Wittig reaction with phosphorus ylids, enabling it to be elaborated into a small library of derivatives, which have shown significant *in vitro* trypanocidal activity.



Profile for Dr. Dhileep Krishnamurthy

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Dhileep Krishnamurthy was born in India and received his M.Sc. degree from Indian Institute of Technology, Bombay. He moved to United States and obtained his Ph.D. degree in synthetic organic chemistry in 1995 under the direction of Professor Gary Keck at the University of Utah, Salt Lake City. During this time he contributed to the total synthesis of anti-tumor antibiotic natural product rhizoxin D and the break through discovery of BITIP catalyzed asymmetric carbon-carbon bond forming reactions.

After a short Post-doctoral stint with Professor Gary Keck, he joined Bristol-Myers Squibb as Research Investigator I. At BMS he was instrumental in discovering the commercial route for anti-viral NCE “Entecavir”. In 1999 he joined Sepracor Inc. at Marlboro, MA as a Principal Research Scientist. At Sepracor, he and his group contributed to number of fast track projects and in 2002 he was named as Associate Research Fellow. In late 2002 he joined Boehringer-Ingelheim where he held various scientific and management responsibilities and in 2009 he was promoted to Director for Chemical development at R & D head quarters in USA. His leadership and mentorship was crucial to provide fast paced identification of cost effective commercial route, practical catalysts for challenging chemical processes, discovery of novel salts and polymorph to support selection of pre-clinical candidates and synthesis of stable and radio labeled isotopes of API and synthesis of glucuronide for DMPK support. In 2011 he moved back to his home country India, where he currently serves as Vice President for R&D in Hyderabad. His research interest includes discovery and development of patent free economical, green, and practical synthesis for biologically active molecules (API) using traditional and modern approaches. He has more than 60 publications and patents. He has delivered invited lectures in many academic institutions and international professional conferences. He is a member of many professional organizations and involved with various advisory committees. Most recently, he served in the judging panel for the USA's presidential green chemistry challenge award.

IL 22

ENABLING GREEN CHEMISTRY AND PROFITABILITY THROUGH EFFECTIVE PROCESS RESEARCH

Dr. Dhillep Krishnamurthy,
Dr. Reddy's Laboratories Ltd., Hydrabad.

For a chemistry based organization such as pharmaceutical company (Generic or Innovator), it is well known fact that the practicing green chemistry directly contributes to profitability and safety. However due to ever increasing complexity of the molecules and increasing regulatory challenges bring various hurdles to alignwith the green chemistry and profitability in the API industry. In this presentation, the effective practices of process research strategies to strengthen the bonding between green chemistry and profitability in he pharmaceutical industries (or any other related organization) will be discussed along with various metrics. During the route selection process (synthetic route design stage) in the API development, incorporation of 12 fundamental green chemistry principles using efficient process research strategies results in green chemisry by design (GCbD).

Abhijit Roychowdhury, Ph.D.

Dr. Roychowdhury earned his Ph.D. from Complex Carbohydrate Research Center, University of Georgia, in 2005. His Ph.D. work focused on the synthesis and biological evaluation of part-structures of peptidoglycan, a bacterial cell wall constituent. He was awarded a graduate research fellowship for his Ph.D.

Following his Ph.D. he spent two years with Sigma-Aldrich Corporation, Saint Louis as a Senior R&D Scientist. Making a transition form organic synthesis to proteomics, at Sigma-Aldrich he lead projects focusing on cell surface engineering for ease of detection of glycoproteins. This was glycoproteomics initiatives, which lead to four new products, presently available from Sigma-Aldrich's catalogue.

He is presently a Sr. Group leader in the Medicinal Chemistry department at Piramal Life Sciences Ltd., where his group is involved in multiple projects in oncology. Presently the group is focusing on new inhibitor design as anti-cancer drugs. He leads a team of highly skilled scientists who focus on optimization of *in-vitro*, *in-vivo* potency of small molecule inhibitors along with their ADMET properties to impart drug-like properties to these new chemical entities. The high-point of his research career in Piramal is the selection of one of his molecules as a clinical candidate for Phase I trial in oncology.

Dr. Roychowdhury has published a total 13 peer reviewed papers in journals of international repute and delivered multiple invited talks.

IL 23

TOXICOPHORES IN DRUG DISCOVERY

Abhijit Roychowdhury, MRSC, Ph.D.
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Multiple drugs have been withdrawn from the market due to various toxicology related issues. This leads to a huge loss of revenue for any pharmaceutical corporation. Thus it has become imperative to design and develop safer drugs. This has prompted medicinal chemists to incorporate safe pharmacophores in the design phase and minimize the chance of toxicity related failure of an otherwise efficacious entity. This talk will deal with various aspects of toxicophores from a medicinal chemist's perspective. It will review the present knowledge base in predicting bioactivations and toxicophores[1,2]. These tricks of the trade can be incorporated during the design phase of any drug discovery program[3].

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IL 24

DESIGNING SPECIFIC DRUGS BY DISRUPTING INTERACTION BETWEEN PREFORMED SIGNALING COMPLEX OF INACTIVE G-PROTEINS AND ADENYLYL CYCLASE ISOFORMS

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In reference to cellular signal transduction, it is the accepted doctrine that heterotrimeric G-protein complexes (Gαβγ) are activated by the binding of a ligand to a receptor. The α and βγ subunits of heterotrimeric G proteins are important regulators of adenylyl cyclase (AC), which controls synthesis of the second messenger cyclic AMP. In the inactive state, the critical effector sites on Gα and Gβγ are not available. When activated, the subunits either dissociate or rearrange to expose these sites to effectors. Recent data shows that Inactive G-proteins (GDP-Gαβγ) exist as a complex with adenylyl cyclase 5 (AC5). G-proteins interact with adenylyl cyclase at two distinct sites; the inactive G-proteins are scaffolded at N-terminus of AC while active G-proteins (GTP-Gαβγ) interact at the catalytic domain of AC. We hypothesize that G-proteins also utilize two different surfaces to interact with the NT versus the activation sites on two adenylyl cyclase isoforms (AC5 and AC6). In support of this hypothesis, mutations within the Gβγ effector surface were tested for Gβγ conditional stimulation of AC5 and for binding to AC5-NT. Although several Gβγ active site mutants are unable to support Gβγ activation, they have no effect on Gβγ binding to AC5-NT. SIGK a competitor inhibitor peptide of Gβγ stimulation has little effect on Gβγ binding to AC6-NT. Furthermore Gβγ binds to the NT of many AC isoforms, suggesting that AC anchoring of heterotrimer may be a common theme for ACs to facilitate GPCR regulation by both α and βγ subunits. We also hypothesize that the existence of preformed signaling complexes play role in fast activation and inactivation of the signaling pathway, generate specificity in signaling. This will be mathematically modeled in terms of affect on rate of formation of cAMP upon disruption of these scaffolded complexes. Finally, the sites responsible of these scaffolding interactions might serve as potential targets for specific drug design that with have fewer side effects.

IL 25

DESIGN, SYNTHESIS, AND BIOLOGICAL EVALUATION OF DGAT1 INHIBITORS AS POTENTIAL ANTI-OBESITY AGENTS

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Department of Medicinal Chemistry**,**

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Obesity is a condition characterized by abnormal or excessive fat accumulation. It is associated with an array of additional health problems including increased risk of insulin resistance, type 2 diabetes, fatty liver disease, atherosclerosis, hypertension, and cardiovascular disease. Orlistat, the only marketed anti-obesity drug, prevents absorption of fat from human diet. However its administration is associated with severe adverse effects such as steatorrhea, fecal incontinence, and urgent bowel movements thereby necessitating the need for newer anti-obesity agents exhibiting fewer side-effects. This has led to the exploration and utilization of newer mechanistic targets, including those that inhibit triglyceride biosynthesis and storage in adipose tissue. The diacylglycerol acyltransferase enzyme DGAT1 presents itself as a potential target due to its involvement in the final committed step of triglyceride biosynthesis. Amino biphenyl carboxylic acids are a known class of potent DGAT1 inhibitors. However a high cLogP and poor solubility of these biphenyl analogs could potentially limit their development. Our efforts have been focused on the design and synthesis of potent DGAT1 inhibitors possessing lower cLogP and improved solubility. The design, synthesis, and biological evaluation of these DGAT1 inhibitors will be discussed.

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Dr. Keshav Deo is presently Vice President – Chemical Research Division at Wockhardt Research Center, Aurangabad. Dr. Deo previously held the positions of increasing responsibilities within the research & development of various Indian pharma companies. He started his carrier from Lupin followed by Tata Pharma, Sun Pharma, Dai-Ichi Laboratories, Ranbaxy and Alembic Limited. Dr. Deo is also life member of various national, international chemical research societies and also recognised supervisor for Ph.D degree in various Indian universities.

Prior to joining Lupin, Dr Deo has completed his Ph.D degree from Central Drug Research Institute, Lucknow, India in 1989 under the direction of Dr.D. S. Bhakuni. He earned his master degree at Agra University, Agra in 1985. His research interests include chemo & regio selective reductions, asymmetric catalysis and insightful process development of significant active pharmaceutical ingredients.

IL 26

ENZYMES AS AN ATTRACTIVE TOOL FOR CHEMICAL TRANSFORMATIONS

Dr. Keshav Deo
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In the 21st century the chemists / biotechnologists are paying attention to carry out the organic transformations as natures do. In other words focus research for obtaining value added products using the cost effective, ecofriendly green tools. The last decay has seen a major transformation in the field of biocatalysis in pharmaceutical industry. Indeed it opens an opportunity to explore the use of enzymes (Nature's tool) as an attractive ways in drug manufacturing organizations. Numerous chiral alcohols / amines are obtained in high enantiomeric purity from the corresponding ketones / imines. Just for discussion take an example of the complex synthesis of vitamin B2. In the past so many years the molecule was manufactured in 8 steps from glucose. But now the same is being manufactured through biocatalysis in two steps. The total production cost has been reduced to 40 % and industrial wastage has been reduced to 95 %. Always the selectivity and reactivity of the enzyme varies to the substrate. The global use during last year is increased by ~20 % against the previous year. I sense an all-pervasive mood of optimism and buoyancy as biocatalysis is reflecting increasingly scientific talent in its use in the large-scale manufacturing. Worldwide companies are struggling with the competing priorities of rising customer's low cost expectations, ever-increasing safety and regulatory burden. Only insightful process development will bring the use of biocatalysis in the lower affordable cost.

IL 27

SULFUR AND NİTROGEN CONTAİNİNG BİSPHOSPHONİC ACİDS ARE A CORNER STONE FOR CALCIUM-RELATED DISORDERS AND THEİR ROLE İN ONCOLOGY

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Jayant Khandare, Ph.D., MRSC

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email: jayant.khandare@piramal.com, khandarejayant@gmail.com

Current Research Position

Senior Research Scientist Drug Discovery, New Chemical Entities- Heading Polymer Chemistry Grp. at Piramal Life Sciences Ltd, Sept. 2009 till date

Research at the interface of macromolecular chemistry, polymer sciences, cancer biology, and imaging. Design and synthesis of highly complex multicomponent systems for capturing cancer circulating cells Design of interactive polymer matrix surfaces for enhanced interactions and cytometry studies PEG-prodrug conjugates for passive cancer targeting, *in vitro* dynamics and *in vivo* cellular imagibility Design of novel gasro-retentive and chronotherapeutic system delivery system with greater hydrodynamicity and buoyancy 02 US Patent Applications filed as a lead scientist, 02 under patent filing

Previous Research Positions

Alexander von Humboldt Experienced Researcher Oct. 2008 - Sept. 2009

Host: Prof. Dr. Rainer Haag, Institut für Chemie und Biochemie, Freie Universität Berlin, Germany

Subject: Macromolecular Chemistry

Post Doctorate Research Fellow March 2008 till Sept. 2008, Institut für Chemie und Biochemie, Germany

Senior Research Scientist Drug Discovery, New Chemical Entities and Polymer Platform Innovations (From 02 Jan. 2007 March 2008); Nicholas Piramal Research Centre, Mumbai

Synthesis of new biopolymers and their modifications for pulsatile drug delivery systems, Synthesis of new biomaterials Preparation of nano-tubes from biopolymers at room temperature

DBT SIBRI-Proposal approved with grant 25 lakhs (grant declined)

Research Associate (Sept. 2004 till Dec 2006)

Dept. of Pharmaceutics, Rutgers, The State University, Piscataway, New Jersey, USA

Advisor: Prof. Dr. Tamara Minko

NIH funding Co PI ($ 1 Million) for anticancer delivery system with homo peptides

Post Doctoral Research Fellow (June 2003 to Aug. 2004)

Advisors: Dr. Mary Lieh-Lai, Children's Hospital, School of Medicine, and Dr. R.M. Kannan, Chemical Engg. and Material Science, Wayne State University, Detroit, MI, USA.

Extensive collaborations with physicians, oncologist and neuro-oncologist at Karmanos Cancer Institute, Ford Hospital, and College of Pharmacy, Wayne State University, MI, USA

Membership and Affiliations

1. Alexander von Humbodlt Experienced Research Fellow
2. Royal Society of Chemistry (RSC)

IL 28

MACROMERS AS TARGETED NANO DELIVERY MATERIALS: OPPORTUNITIES AND CHALLENGES

Jayant Khandare, Ph.D., MRSC
NCE-Polymer Chem. Grp.,
Piramal Life Sciences Ltd. Mumbai, India

Macromolecular and nano-scopic forms of materials are being engineered for delivery of bioactives in the form of prodrug conjugates, depots (liposomes, nanoparticles), polyplexes (complexes), and micelles (self assemblies). The talk will highlight various forms of synthetic polymers and their associated chemistry in tuning for suitable biological applications. Furthermore, the opportunities and challenges in designing such polymeric macromers as multi-component delivery systems in targeting cancer, and *in vitro* and *in vivo* imaging.

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

Paper published in peer reviewed Journals : 96 **Patents (Indian) Filed** : 6

Honors and Awards

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

Member: Editorial Board:

8. Editor- in- Chief: Chemistry & Biology Interface
9. Member of Editorial board , *Future Medicinal Chemistry,Future science group*
10. Member Editorial board , Journal Research and Reports in Medicinal Chemistry
11. Member of Editorial board - Mycobacterial Diseases
12. Member Editorial board ,Global Journal of Organic Chemistry

IL 29

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.
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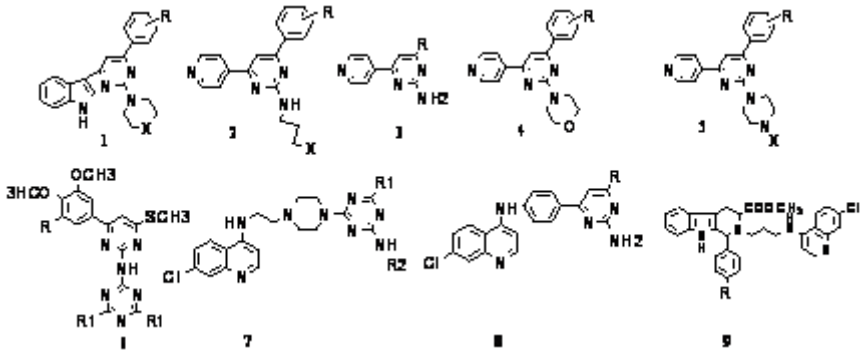
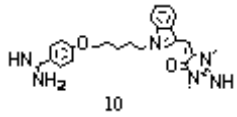
Drug research one of the important area of science. It is also very time taking and require multidisciplinary efforts. Nitrogen heterocycles are constituted a major class of existing drugs. These compounds are widely distributed in nature and are essential to life process.They also play a vital role 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 **1-10** as antiparasitic agents [1-8]. 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.

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Vaidya Jayathirtha Rao

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IL 30

STRUCTURE & SCAFFOLD BASED SYNTHESIS OF HETEROCYCLES AS FAVORED PHARMACEUTICALS: BIOEVALUATION

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Heterocycles form by far the largest of the classical divisions of organic chemistry and are of immense importance biologically, industrially, and indeed to the functioning of any developed human society. Many heterocyclic compounds are biosynthesized by plants and animals and are biologically active. Some heterocycles are fundamental to life, such as haem derivatives in blood and the chlorophyll essential for photosynthesis. Similarly, the paired bases found in RNA and DNA are heterocycles, as are the sugars that in combination with phosphates provide the backbones and determine the topology of these nucleic acids. The biological properties of heterocycles in general make them one of the prime interests of the pharmaceutical industry and biotechnology industry. In this context we have initiated work on the synthesis of heterocycles with an aim to understand their properties towards bioactivity like, antibacterial, antimalarial, antifungal, anti cancer, etc…. We have synthesized nicotinaldehyde skeleton initially and utilized it for making other heterocycles, like qunolines, napthyridines etc.. via Baylis-Hilamn adducts. The results on these aspects will be discussed in detail.

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Teaching Experience	: 27 years
No. of PhD students guided: 53	
Projects Completed	: 05
Project Ongoing	: 05
Under Guidance	: 14
Research Publications	: 100 (National 15, International 85)
Books	: 01
Book Chapter	: 01
Patents (Indian)	: 05

Invited Talks and Chairing of Sessions: 40 (last Five years)

Member: Editorial Board:

1. Journal of Cell and Tissue Research (TRC journal)
2. Medicinal Chemistry: An Indian Journal (Trade Science Incorporation)
3. Associate Editor, Journal of Basic and Applied Pharmaceutical Sciences, Brazil
4. Reviewer of leading National and International journals: Journal of Indian Chemical Society, Bioorganic Medicinal Chemistry, Bioorganic Medicinal Chemistry Letter, Journal of Tissue Research, Arkivok etc.

IL 31

APPROACHES TOWARDS DESIGN AND SYNTHESIS ANTICANCER AGENTS

Prof. Anamik Shah
Principle Investigator:
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Development & Instrumentation Support to Small Manufacturing Pharma Entrprises"
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There are enormous efforts are being carried by medicinal chemists to identify newer scaffolds based on front line "Natural product" like chemical structural architecture especially in the field of anticancer research. The design, synthesis and biological activity of small molecules derived from oxygen and nitrogen containing compounds has played pivotal role in discovering many new anticancer drugs and a fair number of compounds are in preclinical and phase studies. The results from author's laboratory for developing new chemical entities both as anticancer agents and MDR reverting agents will be presented

OP 1

Receptor and Ligand based Design, Synthesis and Biological Evaluation of Peptidic and Non-peptidic Inhibitors of Human Rhinovirus 3C-Protease

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Since the human rhinovirus (HRV) is the most important aetiological agent of the common cold, the last few years have witnessed a growing interest in new effective antirhinovirus agents. The requirement for proteolytic processing of the viral polyprotein, supported by mutagenesis of the active site residues, makes 3C-protease (3CP) inhibitors a suitable target for antirhinoviral therapy[1, 2]. Presently, the known 3CP inhibitors are based on either isatin, benzamide or peptidomimetic scaffolds carrying an □□□-unsaturated ester chain. In order to establish a general structure activity relationship (SAR) model for these rhinoviral inhibitors, three-dimensional quantitative structure–activity relationship (3D-QSAR) analyses as well as docking calculations were performed on the above mentioned benzamide, isatin and peptidomimetic derivatives on the active site of HRV type-2 3C protease[2, 3]. Comparative molecular field analysis (CoMFA) and comparative molecular similarity index analysis (CoMSIA) 3D-QSAR models were developed by using automated docking program incorporated in SYBYL. The obtained results point out that steric and electrostatic feature as well hydrophobicity of the bulky group substituents in these derivatives play a vital role in the overall biological activity and receptor binding. The developed model should be useful for both the design of novel rhinoviral inhibitors and the optimization of the existing ones. Additionally, some new benzamide-based derivatives were synthesized and assayed for cytotoxicity and antirhinoviral activity comparing their features with the reference drugs.

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OP 2

CHARACTERIZATIONS OF THE SUGARS PORTION OF THE ANTIFUNGAL AGENT BY GC-MS STUDY

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The clinical relevance of fungal diseases increases enormously due to the increasing of the immunocompromised host including individuals infected with HIV, transplant recipients and patients with cancer[1,2]. The crude mortality from opportunistic fungal infections still exceeds 50% in most human studies and has been reported to be as high as 95% in bone marrow transplants recipients infected with *Aspergillus spp*. [3] . Furthermore, long-term treatments with commonly used antifungals, such as amphotericin-B have toxic effects: ketoconazole, fluconazole and clotrimazole are limited in their spectrum of pharmacological activity and efficacy and use may result in strain resistance[4]. Recently, we have ascertained the point of linkages between sugar moieties of the sugar portion of the anti fungal agent reported earlier[5, 6] by the interpretation of GC.MS spectra.

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OP 3

EX VIVO EVALUATION OF ROFECOXIB GEL FOR TOPICAL APPLICATION

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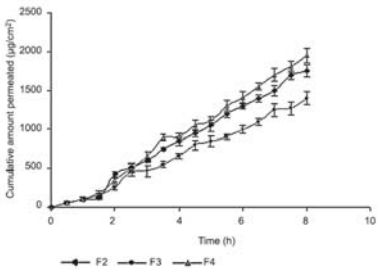
The potential gastrointestinal disorders associated with oral administration of rofecoxib [1] can be attenuated by delivering the drug to the inflammation site at a sustained level over an extended period of time. Hydroxypropylmethylcellulose (HPMC), sodium alginate and Carbopol 940 were used to develop topical gel formulations of rofecoxib. The *in vitro* drug release and *ex vivo* permeation from the gel formulations were examined through cellulose membrane and rat epidermis, respectively, mounting on a Keshary-Chien diffusion cell [2]. The anti-inflammatory activity of the rofecoxib gel formulation was evaluated using the carrageenan induced rat hind paw edema model [3]. The gel formulation consisting of 4% w/w sodium alginate-Carbopol 940 at 3:1 ratio was found to be suitable for topical application based on *in vitro* evaluation and *ex vivo* permeation studies. The drug permeation rate increased with an increase of



Formulations	Percent inhibition					
	1 h	2 h	3 h	4 h	5 h	6 h
Rofecoxib oral	16.66	45.00	52.21	65.51	63.13	62.89
Rofecoxib gel	9.44	35.10	46.34	55.45	56.22	58.93

Fig. 1: Ex vivo permeation from rofecoxib gels. Table 1: Percent inhibitions of hind paw edema.

the initial drug concentration in gels up to 25 % w/w (Fig. 1). An inverse relationship was observed between the *in vitro* drug release rate/*ex vivo* permeation rate and viscosity of the gel formulations. The anti-inflammatory activity of 4% w/w sodium alginate-Carbopol 940 gel containing 25% w/w rofecoxib in the rat hind paw edema model reveals that the drug was delivered to the inflammation site at a controlled level over a period of 6 hours (Table 1). These results suggest the feasibility of the topical gel formulation of rofecoxib.

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OP 4

AMINO ACID-BASED FLUORESCENCE SENSORS FOR DETECTION OF MERCURY (II) IONS

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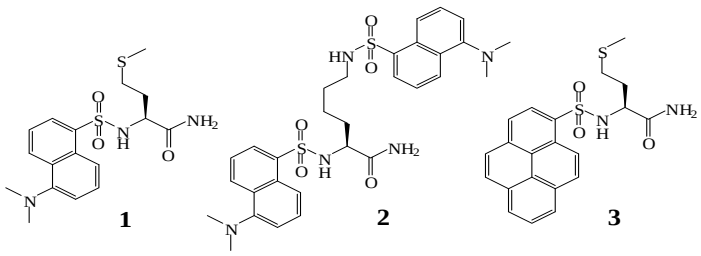
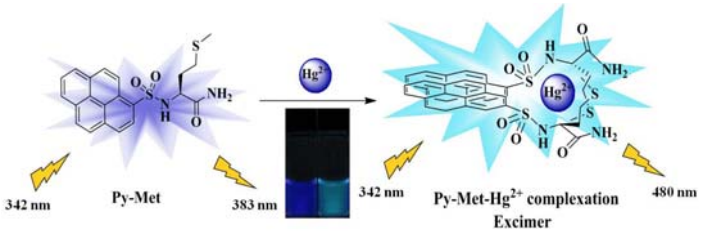
Amino acid-based fluorescent sensors (**1-3**) were synthesized by solid phase synthesis [1, 2]. The compounds (**1-3**) are exhibits highly selective recognition of mercury (II) ions among a series of tested metal ions. The fluorescence behaviors of **1** and **2** showed turn-on response, where as compound **3** exhibit ratiometric response, respectively. Compounds **1-3** are showed highly sensitive to mercury (II) ions without interference of other metal ions. In addition the compound **2** penetrated living HeLa cells and detected intracellular mercury (II) ions.

Hg(II) ions is one of the most toxic metal ions, and its presence in the environment has caused serious problems for human health and ecology [3**]**. The development of selective and sensitive methods for the detection of mercury ions has received much attention. In particular, fluorescence has been regarded as the most powerful optical technique for detecting low concentrations of metal ions, and considerable efforts have been devoted to the development of new fluorescent chemical sensors that detect mercury ions [4–5]. However it is challenging for developing new chemosensors for Hg(II) ions with high sensitivity and selectivity, turn-on or ratiometric response, good water solubility, and cell permeability



1 **2** **3**



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OP 5

COMPARATIVE EFFECTS OF ANTI-HYPERTENSIVE DRUGS-CAPTOPRIL AND ATENOLOL ON SERUM ANGIOTENSIN CONVERTING ENZYME AND ANTHROGENIC LIPID PROFILE IN HYPERTENSIVES.

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Hypertension is the major risk factor of cardiovascular (CAD) disorder. Angiotensin Converting Enzyme inhibitors (ACE-I) and vasodialators such as calcium channel blockers and beta blockers are used as anti-hypertensive drugs. The present study was designed to evaluate the comparative effects of an ACE-I -Captopril and a vasodialator- beta blocker- Atenolol on serum ACE levels and serum lipid profile in hypertensive patients. The hypertensive patients (100) were divided equally in to Captopril Group (before and after treatment) and Atenolol Group (before and after treatment). Blood pressure, blood urea ,serum ACE , creatinine and lipid profile were determined before and after the treatment of both drugs [each 25 mg per day for 30 days]. The results demonstrated that there was a significant decrease in the levels of serum ACE and creatinine as well as blood urea in the hypertensive patients due to the treatment of both the drugs. The anthrogenic lipid profile i.e. the declined serum HDL-C levels and the raised LDL-C levels along with higher CAD risk ratio observed in hypertensives , were also improved due to the treatments of the anti-hypertensive drugs under study. The results suggested that both ACE-inhibitors as well as beta blockers exerted protective and beneficial anti-hypertensive effects by reversing the increased blood pressure, serum ACE levels, anthrogenic lipid profile and impaired renal functions; ACE-I Captopril being more efficient as compared to that of beta blocker- Atenolol. The study indicated that serum ACE levels can help for early diagnosis of hypertensive state.

OP 6

IN SILICO APPROACHES TOWARDS ADDRESSING PROBLEM OF POLYPHARMACOLOGY USING GLYCOGEN PHOSPHORYLASE AND NATURALLY OCCURRING PENTACYCLIC TRITEREPENES AS STUDY MODELS

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Target identification and molecular targeting using chemical entities are the bottle necks in drug discovery. Several bioinformatics tools and molecular docking approaches have enormously contributed to the rational design of cost-effective, efficacious and novel lead molecules. Research over past few decades resulted in the development of virtual screening methods, where several million compounds from various databases can be screened in limited time very effectively. Majority of the investigations performed so far focuses only on a single target ruling out the possibility that the same ligand can bind to an off-target with a high-sequence similarity (especially isozymes) leading to unwanted effects.

Glycogen phosphorylases (GP) are phosphorylase enzymes that are implicated in several metabolic disorders such as type-2 diabetes and also other disease like cancer and coronary disease. GP are present both in muscle and hepatic tissue as isozymes and many inhibitors of GP (GPi) due to lack of specificity cross-react between both these isozymes and lead to delirious side-effects. Taking together the role and features of GP, the objective of the current work is to develop a strategy and set some guidelines in a molecular docking approach in order to develop specific GPi using *in silico* derived pentacyclic triterpenes that can posses reduced cross reactivity.

OP 7

DIRECT ACTIVATION OF C-X BOND OF PYRIDAZINES IN PEG-400 AS ECOFRIENDLY SOLVENT

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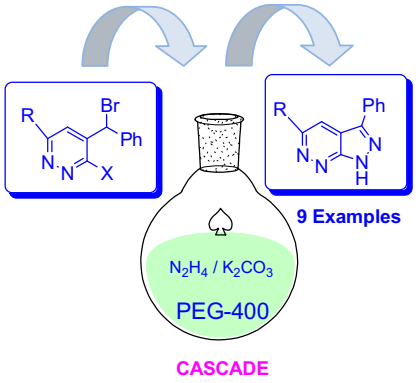
Pyrazolopyridazine is a well known fused ring of heterocycle has shown pronounced biological activity. Besides, pyrazolopyridazine endowed with wide range of analgesic, antimicrobial, anti-inflammatory and antifungal activity. Especially, pyrazolo[3,4-*c*]pyridazine has been identified as a potent inhibition of glycogen synthase kinase (GSK-3) and CDK2/cyclin A. Very few synthetic approaches have been focused on the synthesis of pyrazolo[3,4-*c*]pyridazine. However, these methods have so far as limitation such as lack of selectivity, multistep synthesis, and complexity encountered for the preparation of substrate. Therefore, development of mild and straightforward synthesis of the pyrazolo[3,4-*c*]pyridazine derivatives from readily available starting materials is highly desirable.

Cascade reaction is a significant tool in organic transformation owing to its advantageous aspects towards one-vessel portfolio, consumption of number of step, saving of reagents and solvents and high yield. A direct activation of C-X bond of substituted pyridazine afforded the cascade orientated product, pyrazolo[3,4-*c*]pyridazine has been developed in PEG-400 as a ecofriendly and recyclable solvent. A regioisomer has been successful established by using different bidentated nucleophiles. The reactions were carried out in relative mild condition and PEG-400 could be reused five times with good yield.



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OP 8

CHEMO-SELECTIVE CHEMISTRY TO DESIGN NEW POLY(VINYL ALCOHOL) BASED NETWORKS

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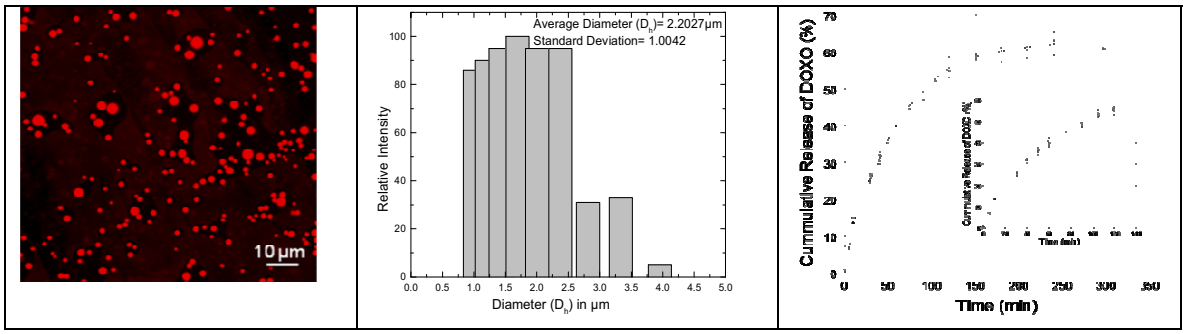
Chemo-selective chemistry represents one of the main synthetic strategies for the design of bioactive matrixes. In this contribution we report on different approaches applied to poly(vinyl alcohol), PVA, based on chemo-selective approaches for the fabrication of novel networks suitable for biomedical applications.

Novel poly(vinyl alcohol), PVA, click microgels were synthesized by inverse emulsion droplets technique (IED). PVA functionalized with pendant alkyne and azide groups were prepared by carbonyldiimidazole (CDI) mediated couplings of amines terminating with different "clickable" functional groups: (i) 11- azido- 3, 6, 9- trioxaundecan-1 amine, (ii) propargylamine. Low degrees (1-5%) of PVA modification were required in order to retain solubility in water. The incorporation of functionalities in the resulting polymer was qualitatively and quantitatively confirmed by FT-IR and proton NMR. Azide-modified PVA and alkyne-modified PVA components were cross-linked by mixing them in the presence of Cu (I), a catalyst for Huisgen's 1, 3-dipolar azide-alkyne cycloaddition. Click of the two differently substituted polymers in IED conditions results in a chemoselective coupling between alkyne and azido functional groups with the multiple formations of triazole cross-links to yield microgel spherical particles. Click chemistry technique was used for surface functionalization of the PVA based microgels. Azido-modified hyaluronic acid (HA), was labeled with fluorescein isothiocyanate (FITC) in order to show the effective coating of the microgel surface by confocal laser scanning microscopy (CLSM). Average diameter of microgel particles was 2µm with narrow size distribution, was evaluated by confocal laser scanning microscopy (CLSM) on a statistically meaningful set of images and hydrodynamic diameter was assessed by dynamic light scattering (DLS). Invitro drug release study carried out using doxorubicin at physiological temperature. Water uptake of microgel is 7.6 ml/g. Size exclusion experiments were performed using fluorescein isothiocyanate-dextran (FITC-Dextran) with different molecular weights for the determination of microgel pore size. Biocompatibility and bioadhesion study carried out on human adenocarcinoma cells.

Chemo-selective methods provide useful synthetic routes for the design of PVA based networks. In combination with IED approach, "Click Chemistry" applied to PVA for the fabrication of microgels spherical particles of potential use as localized drug delivery systems in cancer therapy.



Figures: CLSM image of PVA microgel (Left), Hydrodynamic diameter of microgels by DLS (Middle), Cumulative doxorubicin release from HA coated PVA microgels (right).

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OP 9

OXIDATION OF ALKYL AROMATICS TO AROMATIC KETONES BY TBHP ON NANO AMORPHOUS MnO_2

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Aromatic ketones are key intermediates for the synthesis of insecticides, photo initiators, perfumes and pharmaceuticals and also integral part of various natural products.[1,2] In the recent past, much attention has been paid for the introduction of carbonyl functionality mainly at the benzylic position of the corresponding alkylarenes producing aryl ketones as they are valuable building blocks for numerous specialty chemicals.[3,4] There are some relevant examples including oxidation of Δ^5-steroids to corresponding biologically interesting Δ^5-7-ketone derivative[5] and the benzylic oxidation of xanthene to xanthone.[6]

Traditionally, aromatic ketones are produced by the Friedel-Craft's acylation using homogeneous Lewis acids or strong protonic acids. These processes require critical reaction conditions and stoichiometric amounts of catalysts and also lead to the generation of large volumes of corrosive and toxic waste.[7] In order to develop clean processes various catalytic systems are reported for the synthesis of benzylic ketones. This includes CrMCM-41/H_2O_2,[8] $NaBiO_3$/AcOH,[9] $NaIO_4$/H+/LiBr,[10] $NaClO_2$/NHPI,[11] in situ generated Bi(0) as catalyst / TBHP / picolinic acid, [12]HBr-H_2O_2,[13] $RuCl_2(PPh_3)$-t-BuOOH,[14] Mn(III)salencomplex/iodosobenzene,[15] Co(II)phthalocyanine/[bmim]Br.[16] Presently, industrial production of benzylic ketones is manufactured in presence of molecular oxygen using cobalt cycloalkane carboxylate or cobalt acetate catalyst in acetic acid.[17] Most of these methods suffer from disadvantages like use of corrosive solvents, non recoverable homogeneous catalysts etc. In present work nano amorphous MnO_2 was synthesized by reduction of potassium permanganate using triethanolamine as a reductant and characterized by XRD and SEM techniques. The catalytic activity of the synthesized metal oxide was investigated for the oxidative functionalization of alkylaromatics to benzylic ketones using TBHP as an oxidant. Various manganese oxides were screened, nano amorphous manganese dioxide exhibited significant catalytic activity for the oxidation of alkylarenes selectively at the benzylic position. The nano amorphous MnO_2/TBHP catalytic system provides excellent conversion of alkylaromatics and profitably used up to six consecutive cycles with no considerable loss in catalytic activity.

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OP 10

A FACILE SYNTHESIS OF 3-SUBSTITUTED-2-STYRYL -4-QUINAZOLONES AND ITS BIOLOGICAL EVALUATION

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Quinazolin-4-ones are an important class of compounds and their chemistry continues to be of considerable interest 2-Styryl -4-quinazolones are having similar structure as stilbenzenes, thus they are thought of having biological activity. They are reported as bacterial and fungicidal and also have anti-inflammatory activity along with antimicrobial properties. They are reported to have remarkable pharmacological profile.

The present investigation has been undertaken with a view to studying the possibility of using an amino compound with an aromatic aldehyde, in one pot conversion of suitable O-C=N- heterocycles bearing a methyl group at the imino carbon atom into N-C=N heterocycles having a styryl moiety in places of methyl group. For this purpose 3-substituted 2-styryl-3, 4-dihydro-4-quinazolones were synthesized from N-acetylanthranilic acid. In connection with our studies in heterocycles carrying an activated methyl group, the title reaction was investigated. The synthesis of Substituted 4-Quinlozones is usually carried out in a step-wise fashion (1) , but in the present method, all the steps were carried out in the same flask. Most of the compounds prepared showed a stable yellow color. A series of compounds have been synthesized and their biological evaluation is in progress.

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OP 11

RECYCLABLE CHIRAL CATALYSTS FOR DIFFERENT ASYMMETRIC ORGANIC TRANSFORMATIONS

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The concept of replacing a racemic mixture of biologically active substances with a single enantiomer play a distinctive role in the pharmaceutical, agrochemicals, flavor and fragrance. The reason for this development is that the enantiomers often exhibit different biological activities. Therefore, the performance of the single enantiomer usually is superior to that of the racemic mixture. Among the different methods for producing enantiomerically pure compounds, asymmetric catalysis is an excellent strategy since a small amount of a chiral catalyst can be used for producing thousands of chiral products. Although highly selective catalysts have been found for a large number of catalytic transformations, there are only a few general catalytic systems that are enantioselective for a wide range of reactions and substrates. Moreover, it is difficult to predict which catalyst that will be the best for a given target molecule. Therefore, the designing of the catalyst as well as the reaction conditions usually need to be optimized for each particular transformation. Our efforts in designing of chiral metal complexes for the synthesis of enantio-pure epoxides and their derivatives as key intermediate for pharmaceuticals will be presented.

OP 12

SYNTHESIS OF 2-SUBSTITUTED[1,2,4]-TRIAZOLO[3,2-C][1,3,5]-THIADIAZINE3, 3-DIOXIDES

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Fused 1,2,4-triazole represent an interesting class of compounds due to their versatile biological activities and their synthesis has attracted the attention of several synthetic groups[1]. Some times the fusion of heterocyclic nuclei enhances the biological profile manifold more than its parent nucleus [2]. The 1, 3, 5-thiadiazine and its derivatives are reported to be insecticidal and accaricidal activity [3-8]. These compounds are also reported to possess antifungal [9-10], hyplopemic [11] and antiatherosclerotic activity [12]. The triazolo-thiadiazines are reported to be antimicrobial, antibacterial, anticancer [13] and diuretic activity [14]. These diverse biological activity prompted us to synthesise some [1,2,4]-triazolo[3,2-c]1,3,5-thiadiazine-3,3-dioxide derivatives with the expectation of enhancing the biological activities of these class of compounds. The title compounds were synthesized from 3-benzylidineamino-[1, 2, 4]-triazole [15] and sulfene generated *in situ* by a [4+2] Diels-Alder Cycloaddition reaction. 2-substituted[1,2,4]-triazolo[3,2-c]-thiadiazine3,3-dioxide derivatives were successfully synthesized by the dropwise addition of methanesulfonyl chloride in dioxane to a solution of 3-benzylidineamino[1,2,4]-triazole in dioxane at 0-5^{0}c under stirring during 30 min. The stirring was continued for a period of 3-4 hour at the same temperature. The reaction mixture was then poured into ice and extracted with chloroform and dried over anhydrous Na_2SO_4.The solvent was removed under reduced pressure and recrystallization of the residue gave the title compounds. All new compounds were characterized from ^{1}H NMR,IR, MS spectra and elemental analysis.

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OP 13

Nanotechnology: Beginning of a New Era in the Medical Sciences

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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 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 exhaustively inventory cells, cell parts, and molecules within cell parts to answer questions such as, "How many?" "How big?" and "How fast?" Obtaining thorough, reliable measures of quantity is the vital first step of this needs a lab to be established with a few nano medicine centers. These centers will have experts of highly interdisciplinary scientific caliber including biologists, physicians, mathematicians, engineers and computer scientists to design a particular strategy in fighting against diseases.

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 science.

OP 14

RECYCLABLE Cu(II)-MACROCYCLIC [H_4]SALEN CATALYZED HENRY REACTION FOR THE SYNTHESIS OF VALUABLE DRUG (*R*)-ISOPROTERENOL (□-ADRENORECEPTOR)

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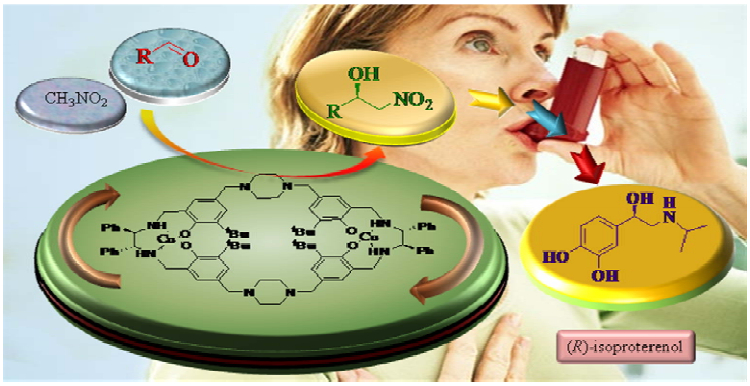
The asymmetric nitroaldol reaction has emerged as a powerful synthetic tool for the stereoselective C-C bond forming reaction because the resultant *β*-hydroxy nitroalkanes are important building blocks for the preparation of *β*-amino alcohol derivatives, α-hydroxycarboxylic acid and *β*-receptors [1,2]. In this direction various chiral metal complexes with BINOL, aminoalcohol, bis-(oxazoline), bis-(thiazoline), bis-(imidazoline), sulfonylamine, salen, Schiff bases, thiols, thiophene, bipiperidine, aminopyridine, oxabispidine and organocatalyst have been reported for asymmetric Henry reaction under homogeneous system. Among them Schiff base ligands have been recognized as 'privileged ligands' because they can be easily prepared through the condensation between various aldehydes and primary amines [3]. Due to the more solubility of the chiral catalyst in reaction medium, their separation and recyclability is problematic. Therefore, C_2-symmetric dimeric [H_4]salen ligands with two active centers derived from piperazine-bis aldehyde and 1*R*,2*R*-(-)-1,2-diphenyl-1,2-diaminoethane were synthesized in order to recycling the catalyst systems for Henry reaction and also to avoid high catalyst loading, sensitivity to air or moisture, and narrow substrate variation with $Cu(OAc)_2.H_2O$ as metal source. The catalysts were effectively recycled up to five cycles with preservation of its catalytic activity and enantioselectivity. We have also made use of the alternative route (via asymmetric Henry reaction) for the synthesis of (*R*)-isoproterenol as a potent □-adrenoreceptor for bradicardia or heart block. It is also a highly effective bron-chodilator and therefore, used in the treatment of asthma and chronic obstructive pulmonary diseases.



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OP 15

ORGANOCATALYTIC DIRECT ALDOL REACTION: GREEN APPROACH TOWARDS THE SYNTHESIS OF AMINO-POLYOLS

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Organocatalysis has grown-up rapidly and applied successfully to several different enantioselective reactions in last few years. In particular, the direct asymmetric aldol reaction catalyzed by small organic molecule (L-Proline) is the great breakthrough in this field of research.[1] Amino-polyols are important building blocks for several important natural and unnatural products of biological importance. In particular, nitrogen analogous of carbohydrates, known as azasugars are of great importance as they exhibit significant glycosidase inhibitory activity.[2] Recently, we have developed highly diastereoselective intermolecular aldol reaction of ketones with various amino-aldehydes catalyzed by L-Proline **1** as organocatalyst.[3] The corresponding aldol product was further transformed into long chain amino-polyols (Scheme 1a). Similarly, a new general strategy for the synthesis of azasugars, using intramolecular diastereoselective aldol reaction catalyzed by L-Proline was established (Scheme 1b).[4] Details of the concept, design and synthetic strategy will be presented here.

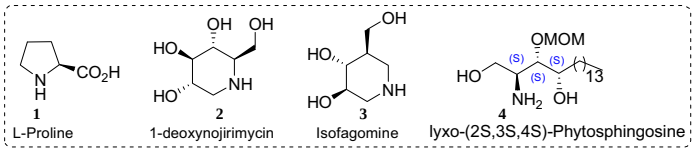
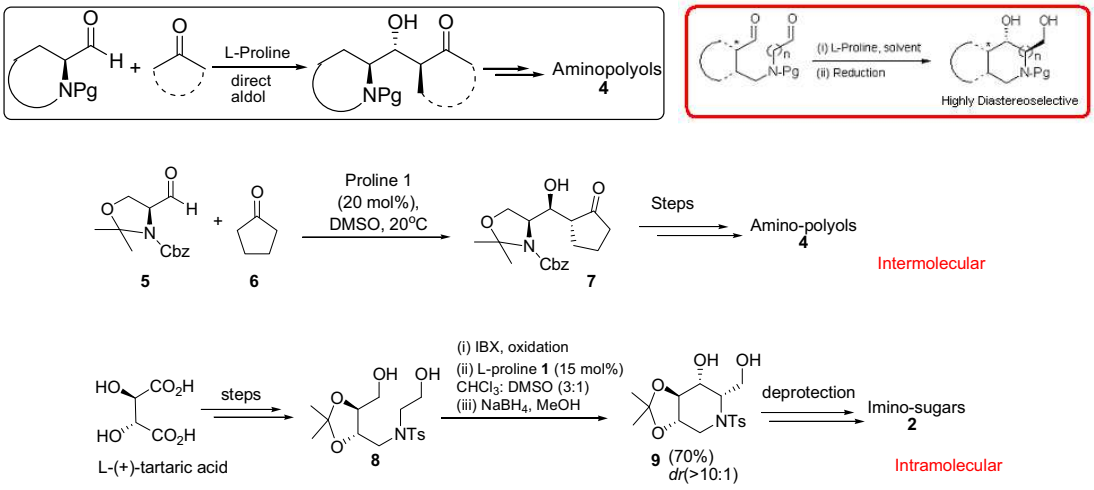


Figure 1: Proline **1** and selected amino polyols



Scheme 1: Inter and Intramolecular direct diastereoselective aldol reaction catalyzed by L-proline as synthetic approach for the synthesis of amino-polyols

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PP 1

FACILE SYNTHESIS OF PYRANO STEROIDS VIA D-RING CLEAVAGE

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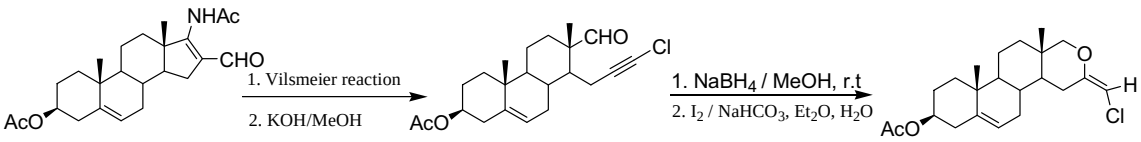
Heterosteroids are gaining much importance in the recent years for their profound biological activities. The biological activities of heterosteroids are mainly due to the fusion of a heterocyclic ring to the steroidal moiety. Modifications of steroidal D-ring have attracted great attention of medicinal chemists for their pharmaceutical properties. D-ring annelated heterosteroids like Abiraterone, and 17-imidazolyl steroids have already been reported to exhibit biological activities against prostate cancer, which is one of the leading causes of cancer-related mortalities in men [1]. The steroidal β-formyl enamides has shown enormous potential in the preparation of D-ring annelated heterosteroids and des-D steroids [2]. The β-formyl enamide moiety has been conveniently employed in inverse electron demand Diels-Alder reaction [3], Vilsmeier reaction [4] and geminal dichloride formation reactions [5]. In continuation of our interests for developing newer heterosteroids, herein, we report an efficient methodology for the synthesis of pyrano-steroid from β-formyl enamide via D-ring cleavage.



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PP 2

PHYTOCHEMICAL CONSTITUENTS AND BIOLOGICAL ACTIVITIES OF CURCUMA LONGA

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Curcuma longa L. Syn *C. domestica* Val. ('Haldi') family Zingiberaceae is extensively cultivated for its rhizomes, which are dried, powdered and used as turmeric. It is a perennial herb distributed throughout tropical and sub-tropical regions of the world like India, Pakistan, Bangladesh and Sri Lanka. Its rhizomes are harvested, washed and boiled in mild alkaline water to soften and dried in sun or in electric driers. It is used as coloring matter in pharmacy, confectionery, food industry, for dyeing wool, silk, cotton and in combination with other natural dyes to get different shades. Rhizomes are used as cosmeceutical, expectorant, antiseptic, anthelmintic, blood purifier, in leprosy, spleen disorders, rheumatism, bronchitis, cough and cold, insecticide, spasmolytic, hypotensive, cholera and syphilis. It is also an ingredient of 'Ayurvedic' drug for malarial fever; indigenous antifatigue drug Geriforte (Geri Care/Stress Care), Unani drug Majnoon-E-Falsfa, Vitafix, Opthacare, Purime (Hemo Care), V-Gel, Fem Care Gel, Acne-n-Pimple Cream, Anti-Wrinkle Cream, Blood purifier Capsules and Syrup, Foot care Cream, Dibecon (Gluco Care), Curcumin-97 and Curcumin 900 MG. In the modern pharmaceutical products it is an ingredient of 'Geriforte' effective in senile pruritis, insecticide, spasmolytic, hypotensive, antifungal, anti-inflammatory, antibacterial and to fight decaying metabolism to prevent cancer. It is widely used as spice, preservative, coloring matter and has wide range of medicinal and pharmacological activities. It exhibits anti-human immunodeficiency virus, anti-bacteria, antioxidant, nematocidal, anti-parasitic, antispasmodic, anticarcinogenic activity. It is a potent scavenger of a variety of reactive oxygen species including superoxide anion, hydroxyl radical, singlet oxygen, peroxynitrite and nitric oxide. It is an inhibitor of ROS generating enzymes cyclooxygenase and lipoxygenase and plays active role in the inhibition of COX-I and COX-II enzymes that involve in the inflammatory reaction. The turmeric extracts protect lipids, haemoglobin, red blood cells from lipid peroxidation induced by hydrogen peroxides. Safety evaluation studies indicate that the turmeric is well tolerated at a very high dose without any toxic effects. Curcumin is one of its major components responsible for its various biological actions. Pure curcumin has more potent superoxide anion scavenging activity than demethoxycurcumin or bisdemethoxycurcumin. Curcumin acts as a pro-oxidant in the presence of transition metal ions (copper and iron) and is a potent bio-protectant with a potentially wide range of therapeutic applications.

PP 3

ROLE OF PHYTOESTROGENS ENRICHED NUTRACEUTICALS FOR THE PREVENTION AND TREATMENT OF OSTEOPOROSIS

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The nutraceuticals comprises bioactive phytochemicals that protect or promote health and occur at the intersection of food and pharmaceutical industries. Plants with estrogen-like biological activity are being used in traditional systems of medicine and folklore. Estrogen is the generic term for chemically similar family of substances that function endogenously as hormones affecting female reproductive function and/or anatomy and play an important role in maintaining bone mineral density by regulating the formation and resorption of bone. Since lower circulating estradiol levels are found during menopause, calcium is lost from the bone into blood plasma, leading to osteoporosis. Hormone replacement therapy (HRT) stimulates bone formation and may prevent bone loss, osteoarthritis and incidence of osteoporosis in postmenopausal women. However, if taken alone, HRT can increase the risk of developing ovarian, uterine and breast cancer.

Phytoestrogens are non-steroidal phytochemicals quite similar in structure and function to gonadal estrogen hormone. They offer an alternative therapy for HRT with beneficial effects on cardiovascular system and may even alleviate menopausal symptoms. They are potential alternatives to the synthetic selective estrogen receptor modulators (SERMs), which are currently applied in HRT. Apart from their estrogenic properties they are also have antioxidant effects due to their polyphenolic nature, anti-carcinogenic, modulation of steroid metabolism or detoxification enzymes, interference with calcium-transport and favorable effects on lipid and lipoprotein profiles. On the basis of chemical structure, phytoestrogens can be classified as flavonoids, isoflavonoids, coumestans, stilbenes, lignans and terpenoids. Isoflavones have the capacity to act like an estrogen and provide health benefits. Soybean is rich in isoflavones like genistein, daidzein and their methyl ether derivatives, biochanin A and formononetin. Consumption of these in high quantities is associated with reduced risk of osteoporosis and related health problems. Coumestrol and 4′-methoxy-coumestrol are two potent members of coumestans mainly found in sprouted legumes. Secoisolariciresinol and matairesinol are two lignan dimers, which are not estrogenic by themselves, but readily convert to the mammalian lignans, enterodiol and enterolactone, respectively and have estrogenic, antiviral, antifungal and antioxidant activities. Terpenoids (ferutinine, tschimgine, and tschimganidine) found in the Umbelliferae family have estrogenic activities. Ferutinine and tschimganidine are sesquiterpenoids and tschimgine is a monoterpenoid. In female's life is affected by a variety of estrogen-related conditions such as osteoporosis, cognitive and cardiovascular decline, increased risk of breast cancer and other symptoms that decrease the overall quality of life. Phytoestrogens (PE) are effective in maintaining bone mineral density (BMD), prevent bone loss, and help in the prevention and/ or treatment of such health related problems. Diet rich in plant-derived products may supply a variety of PE capable of producing a range of pharmacological effects and protection from various diseases. Postmenopausal women who have the greatest risk of breast cancer should be encouraged to increase intake of PE, which is associated with reduced risk of osteoporosis and related health problems.

PP 4

SYNTHESIS OF D-RING ANNELATED AZA HETEROCYCLES: STUDIES ON SOLVENT EFFECT

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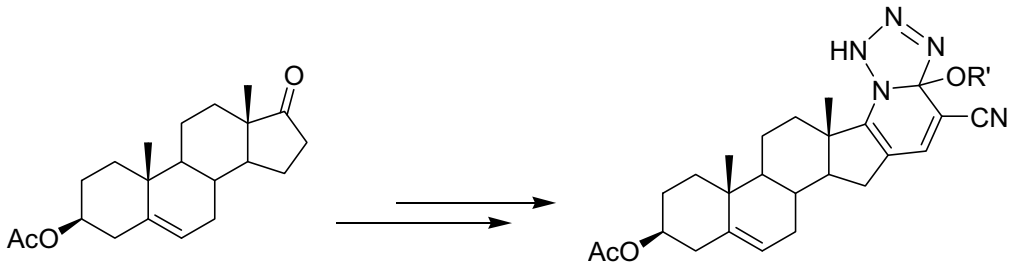
The existence of a large number of pharmaceutically active aza heterocyclic compounds obtained from natural and synthetic sources have provided much scope for their systematic study. The aza heterocycles annelated to steroidal moiety also play a vital role towards important discoveries in medicinal chemistry [1]. The azasteroids find importances as drugs for various ailments. The A- ring and D-ring annelated heterosteroids viz. Finasteride, Danazole and Cortivazole are well known drugs against Benign Prostatic hyperplasia, Breast cancer and bone marrow cancer respectively. D-ring annelated heterosteroids such as Abiraterone also show excellent biological activity against Prostate cancer, which is one of the leading causes of cancer related mortality in men [2]. We have earlier modified some novel strategies for the synthesis of A- and D- ring annelated steroidal aza heterocycles from various semi synthetic steroidal compounds [3, 4]. Herein we present synthesis of newer aza heterosteroids by molecular modification of steroidal rings.



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PP 5

POTASSIUM FERRO-CYANIDE CATALYZED AN EFFICIENT AND CONVENIENT SYNTHESIS OF BENZOXAZOLES AND BENZOTHIAZOLES

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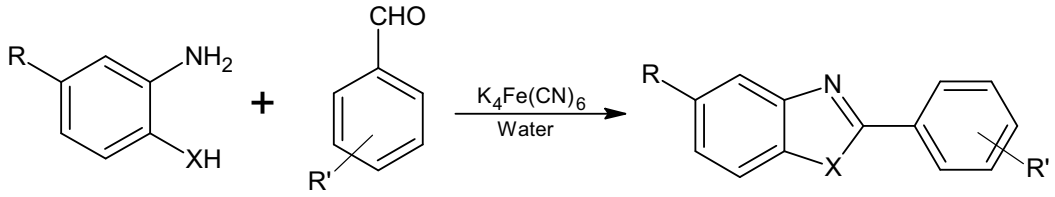
Benzoxazoles and benzothiazoles are very important group of heterocyclic compounds that have many applications in both pharmaceutical and industrial research. They are widely found in bioorganic and medicinal chemistry with applications in drug discovery such as antitumour, anticonvulsant, and antiviral applications.[1-3] Because of these potent biological activities, the research still continuous to have a better methodology for the synthesis of benzoxazoles and benzothiazoles in terms of simplicity, eco- friendly and economic viability, which is achieved by using Potassium ferro-cyanide.

The metal co-ordinate complex $K_4[Fe(CN)_6]$ is an efficient and environmentally benign catalyst[4-6] used for the synthesis of benzoxazoles and benzothiazoles from various aldehydes and o-aminophenol/o-aminothiophenol in aqueous medium at room temperature. This protocol gives excellent yield of products with desired purity.



Scheme: Synthesis of Benzoxazoles and Benzothiazoles

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2. S Hays, J M J Rice, D F Ortwine, G Johnson, R D Schwarz, D K Boyd, L F Copeland, M G Vartanian and P A J Boxer, Pharm. Sci. 83, 1994, 1425.
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PP 6

STANNOUS CHLORIDE AS AN EFFICIENT CATALYST FOR THE SYNTHESIS OF 1,5-BENZODIAZEPINE DERIVATIVES UNDER SOLVENT FREE CONDITIONS

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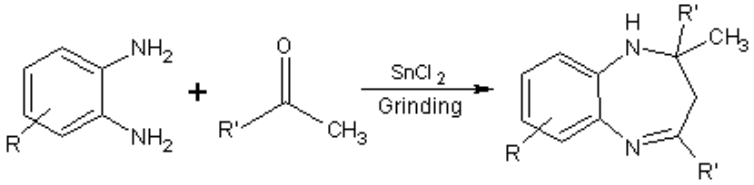
Benzodiazepines have recently attracted attention as an important class of heterocyclic compounds in the field of drugs and pharmaceuticals. These compounds are widely used as anticonvulsant, antianxiety, analgesic, sedative, antidepressive, hypnotic agents [1-4] as well as anti-inflammatory agents. [5] Other than their biological importance, benzodiazepine derivatives are also commercially used as dyes for acrylic fibers. [6] Moreover, 1,5-benzodiazepine derivatives are valuable synthons that can be used in the preparation of other fused ring compounds such as triazolo-, oxadiazolo-, oxazino-, or furano-benzodiazepines. [7-10] As a result, research in this area is still very active and is directed toward the greener synthesis of compounds with excellent yield. In recent years, Stannous Chloride is frequently used in organic synthesis [11] as a catalyst due to its properties such as nontoxic nature, easy availability, inexpensiveness and easiness for work up. Various biologically important 1,5-benzodiazepine derivatives were efficiently synthesized in excellent yields using catalytic amounts of Stannous Chloride (10 mol %). This inexpensive, nontoxic, and readily available catalyst efficiently catalyzes the condensation of several aromatic ketones with substituted o-phenylenediamines.



Scheme: Synthesis of 1, 5-benzodiazepines

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PP 7

POTASSIUM FERRO-CYANIDE CATALYZED HIGHLY RAPID SYNTHESIS OF BENZOXAZOLES AND BENZOTHIAZOLES UNDER SOLVENT FREE CONDITION

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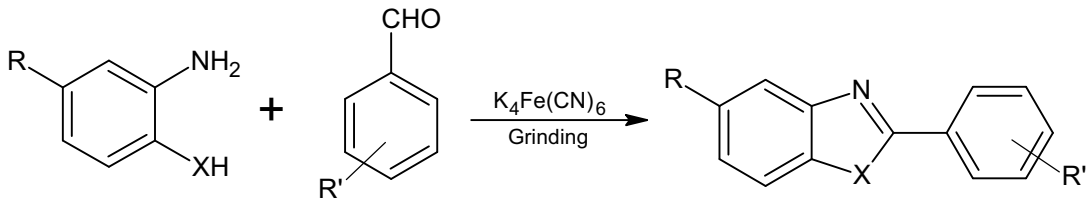
Benzothiazoles and benzoxazoles are very important group of heterocyclic compounds that have many applications in both pharmaceutical and industrial research. They are widely found in bioorganic and medicinal chemistry with applications in drug discovery such as antitumour, anticonvulsant, and antiviral applications.[1-3] They have also found applications in industry as antioxidants, vulcanization accelerators, and as a dopant in a light-emitting organic electroluminescent device.[4,5]

Due to their wide range of pharmacological activity in synthetic and industrial applications, the synthesis of these compounds has recently received a great deal of attention for the discovery of improved protocols towards milder and high yielding approaches.



Scheme: Synthesis of Benzoxazoles and Benzothiazoles

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PP 8

AN EXPEDIENT SYNTHESIS OF A LIBRARY OF SCHIFF`S BASES AND THEIR ANTIMICROBIAL STUDIES

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A library of Schiff bases have been synthesized by the reaction of substituted hydrazones and halo substituted aromatic aldehydes via solution reaction at room temperature. The promising feature of this reaction is very short reaction time (a couple of minute) and excellent yield with high purity. These newly synthesized molecules have been established on the basis of physical, chemical and spectral studies and further screened for their antimicrobial potencies which reflect moderate to good activity against different pathogens.

PP 9

NATURAL PRODUCTS FROM BIODIVERSE ORGANISMS IN DRUG DISCOVERY

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In recent years, natural products from biodiverse organisms have yielded a considerable number of drug candidates. Curacin A is a potent, anti-mitotic algal natural product obtained from strains of the tropical marine cyanobacterium *Lyngbya majuscula*. It exerts its potent cell toxicity through interaction with the colchicine drug binding site on microtubules and inhibits tubulin polymerization in cells. Dolastatin 10, isolated from the Indian Ocean sea hare *Dolabella auricularia*, is a natural, cytotoxic peptide with microtubule-inhibitory and apoptotic effects. The dolastatin family also possesses anti-neoplastic, bactericidal and fungicidal properties. The structurally-related γ-lactams salinosporamide A, omuralide and lactacystin, of bacterial origin, inhibit proteasome activity and are of interest as lead compounds for the development of anticancer agents. Salinosporamide A, a novel marine natural product, produced by an obligate marine bacterium *Salinispora tropica*, found in ocean sediment, is a potent proteasome inhibitor used as an anticancer agent. Squalamine lactate, a novel anti-angiogenic aminosteroid, isolated from the dogfish shark *Squalus acanthias*, is targeted for the treatment of ovarian cancer. Bovine lactoferrin, an antimicrobial component of colostrum and milk, helps in the protection of infants from gastrointestinal infections. Porcine pepsin cleavage of native lactoferrin produces low molecular weight peptides inhibitory to some Gram-negative and Gram-positive bacteria. Hydrolysis of native lactoferrin at pH 2 and 120°C produces active peptides that are bactericidal.

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PP 10

COMPARATIVE ANTIMICROBIAL STUDY OF CLOVE OIL & ITS EXTRACT FOR ITS ROLE AS BIO-PRESERVATIVES

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A comparative study was carried out on the antimicrobial activity of clove oil and its extract prepared in 50%v/v ethanol for their role as natural antimicrobial agents on some selected food spoilage bacteria. The antimicrobial activity was tested against ten bacteria (seven Gram positive & three Gram negative) and seven fungi commonly associated with food spoilage by agar well diffusion assay. The clove oil was found to be better antagonistic agent as compared to its extract counterpart by inhibiting both the groups of bacteria and fungi. The oil produced inhibition zones of diameter (IZD) ranging between 15-24mm and produced widest zone against *Bacillus cereus* and *Listeria monocytogenes* with an IZD of 24.0mm and 21.0mm respectively and a lowest minimum inhibitory concentration (MIC) of 2.5% (v/v). The fungi, *Aspergillus Niger* followed by *Penicillium sp.* was found to be highly sensitive to the oil with an IZD of 42.0mm and 40.0mm respectively and a lowest minimum inhibitory concentration of 2.5% (v/v) for each fungal species. On the other hand, for clove extract inhibition zones against bacteria ranged between 12.0- 26.0nm and for fungi between 20.0- 30.0mm. Sodium propionate (standard food preservative) was used as a positive control in the present study. Clove oil was found to be a better antagonistic agent as compared to both clove extract and standard preservative. This study shows clove oil to be a promising candidate as a future bio-preservative.

PP 11

COMPARATIVE STUDY OF SYNTHESIS, CHARACTERIZATION, ANTIMICROBIAL STUDY OF TI (IV), ZR (IV) AND HF (IV) SCHIFF BASE COMPLEXES

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The synthesis of transition metal complexes of Ti(IV), Zr(IV) and Hf(IV) are derived from schiff base ligands (1,2) obtained by the condensation of aromatic aldehyde and substituted benzoic acid. These compounds are having industrially important application as insecticidal and antimicrobial properties(3-5). These prepared compounds were characterized by using IR and UV-VIS spectroscopy. The determination of the antimicrobial activity of the ligands and of the complexes was carried out on samples of gram positive ***Staphylococcus*** spp. and ***Enterococcus fecalis*** and in gram negative ***Escherichia coli, Pseudomonas perumonia*** and ***Salmonella typhi***. The antimicrobial activity test results proved that all the prepared complexes are active.

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PP 12

SYNTHESIS, SPECTRAL, MAGNETIC SUSCEPTIBILITY STUDIES ON SYMMETRICALLY SUBSTITUTED METAL (II) NITROPHENYL METHANIMINE PHTHALOCYANINE

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Present paper discuss the synthesis and characterization of metal (II) 1, 3, 8, 10, 15, 17, 22, 24-octa-1-(3-nitrophenyl) methanimine phthalocyanines (M-NPhImPcO) (M = Cu, Co, Ni, Zn) by an efficient simple, and novel method. Octaamino metal (II) phthalocyanines were synthesized by the reduction of the corresponding nitro phthalocyanines. The dark green octa-1-(3-nitrophenyl) methanimine phthalocyanine derivatives were characterized by elemental analysis, magnetic susceptibility, electronic, IR and powder X-ray diffraction studies to check the purity, structural integrity and crystalline properties of the complexes. Magnetic susceptibility studies on Co (II) and Cu (II) octa-1-(3-nitrophenyl) methanimine phthalocyanine complexes exhibit a variation of the magnetic moments as a function of field strength indicating the presence of inter molecular co-operative effect. The title complexes were screened for antifungal activity.

PP 13

DESIGN, SYNTHESIS AND EVALUATION OF NOVEL QUINOLINYLPYRIMIDINE DERIVATIVES AS ANTIMICROBIAL AGENT

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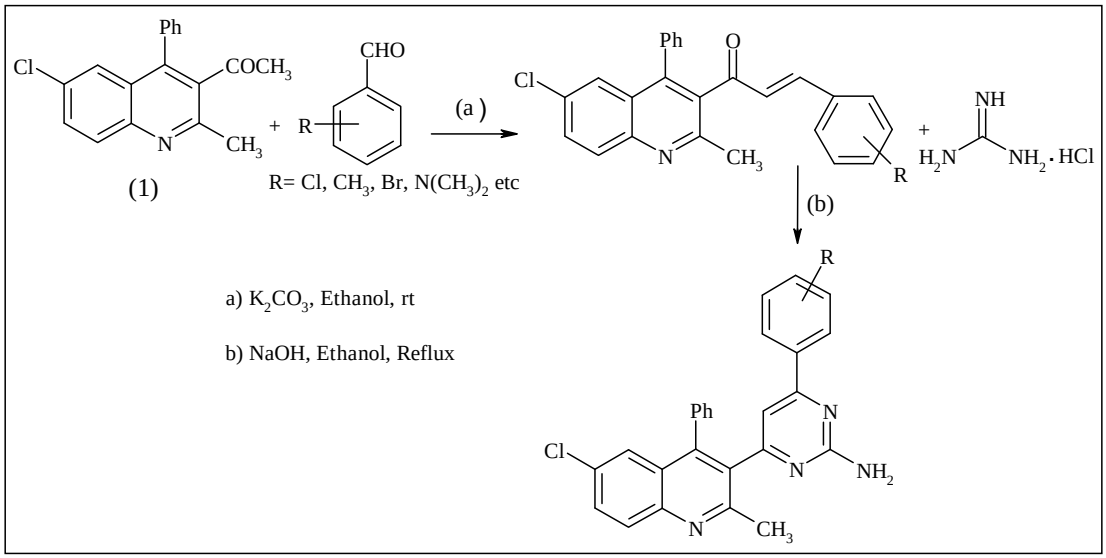
Heterocycles are abundant in nature and are of great significance to life because their structural subunits exist in many natural products, as well as in pharmaceuticals, dyes and many more compounds. Hence, they have attracted considerable attention in the design of biologically active molecules. Quinolines are frequently occurring motifs in medicinally relevant compounds and on the other hand pyrimidine scaffold is a fundamental part of nucleic acids and has been associated with number of biological activities. If pyrimidine and quinoline moiety clubbed into one molecule, the resultant molecule may enhance the pharmaceutical activity up to some extent. Hence, it was thought proper to explore the study of such molecules.

Here, we report two step synthesis of new prototypes by combining both pyrimidine and quinoline moiety starting with quinolinyl chalcones as a source of α, β-unsaturated ketones and guanidine hydrochloride as nucleophile in basic media under refluxing conditions. All the synthesized compounds were evaluated for their antimicrobial activity against different strains of bacteria and fungi.Most of the tested compounds showed moderate to good antimicrobial activity.



Scheme-I

PP 14

A NEW SYNTHESIS OF β -ANILINO-CHALCONES BY REGIOSELECTIVE OXIDATION OF β -ANILINO-DIHYDRO-CHALCONES USING IODINE-DMSO

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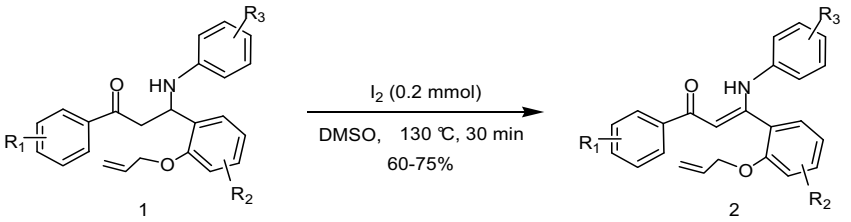
β-Enaminones are important precursors of a wide variety of heterocycles [1] and pharmaceutical compounds [2]. They exhibits anti-epileptic, molluscicidal, and larvicidal activities and employed as an intermediates for the synthesis of naturally occurring alkaloids [3]. β-Enamino ketones were widely applied in the functional group transformation in the field of organic chemistry, including β-alkoxyvinyl ketones enamination, 1,2-aryl migration, 1,3-dicarbon enamination, imidoyl chlorides with lithium enolates of alkyl propanoates to β-enaminones, lithiate enamine acylation and Sonochemical Blaise reaction. These synthetic routes involve cyclic β–enaminones as well as β-anilino chalcones synthesized in the present work. Due to the importance of β-enaminones as valuable biologically active compounds, a simple and efficient approach for this transformation is highly desirable.

β-Anilino-dihydro-chalcones were prepared from aromatic aldehydes, substituted acetophenones and anilines by Mannich reaction using ammonium chloride as an inexpensive and readily available reagent. β-anilino-dihydro-chalcones readily undergo oxidation at aliphatic region in presence of catalytic amount of iodine in dimethyl sulphoxide at 130 °C in high yield. Oxidation of allyloxy substituted β-anilino-dihydro-chalcones to β-anilino-chalcones is a preferred reaction over deallylation.



1 2

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PP 15

SYNTHESIS OF NEW PYRAZOLINES, ISOOXAZOLINES AND THIOPYRIMIDINES BEARING THIAZOLYL AND ETHERAL PHARMACOPHORE

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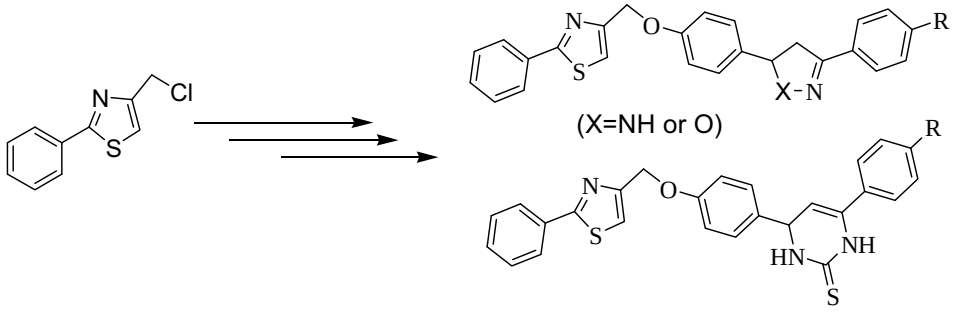
Derivatives of pyrazoline, isooxazoline and thiopyrimidine have played crucial role in the development of heterocyclic chemistry and have been used extensively as an important pharmacophores and synthones in the field of medicinal chemistry. Many classes of chemotherapeutic agents are having pyrazoline, isooxazoline and thiopyrimidine nuclei and these are in clinical use. Pyrazoline, isooxazoline and thiopyrimidine scaffolds have also been found as key cores in various antidiabetic drugs. Ethereal linkage is essential component in the molecular framework of various antidiabetic agents like rosiglitazone and pioglitazone. The thiazole ring unit is also a common structural feature in various bioactive molecules.

In view of the pharmacological importance of pyrazolines, isooxazolines, thiopyrimidines, thiazoles and ethereal linkages, here it was thought worthwhile to construct some new pyrazolines, isooxazolines and thiopyrimidines each with thiazolyl and ethereal pharmacophores with the hope to obtain the compounds with intensified bioactivities.

Therefore here we report and present our attempts, made to construct the desired new heterocycles starting from 2-phenyl-4-chloromethyl thiazole by developing convenient and sustainable synthetic routes. The details of the synthetic work and structural elucidation of the intermediates and the desired products will be presented (**Scheme I).**



Scheme I

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PP 16

SYNTHESIS AND ANTIOXIDANT, CYTOTOXICITY AND ANTIMICROBIAL ACTIVITIES OF NOVEL CURCUMIN MIMICS

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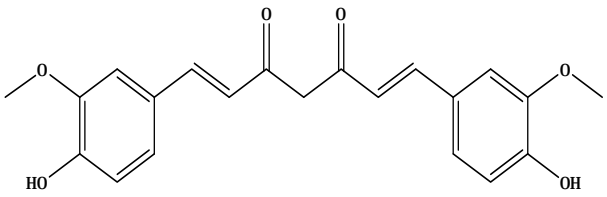
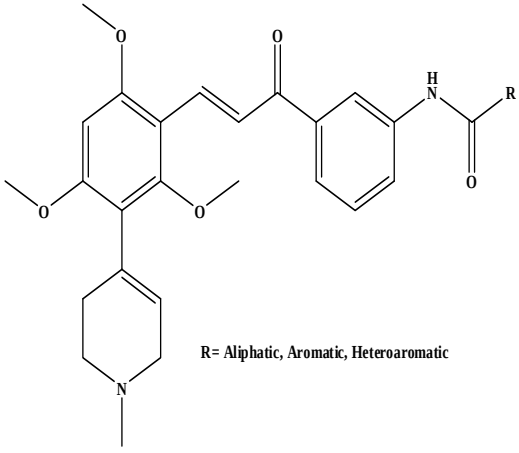
Curcumin is a β-diketone constituent of the turmeric that is obtained from the powdered rhizome of *Curcuma longa*. Curcumin has a wide range of interesting biological activities such as anti-inflammatory, antioxidant, antiviral, cutaneous wound healing, hypocholesterolemic effects in diabetic patients, anti-angiogenic and stimulatory response to stress-induced biological activity [1,2]. Although curcumin is non-toxic and has promising biological activities, clinical studies indicate its poor bioavailability and pharmacokinetic profile. To overcome these barriers several research groups have synthesized curcumin analogues. We herein report on the synthesis of the novel curcumin mimic incorporating olefin as well as aromatic, alicyclic or heteroaromatic amide moieties.

Claisen-Schmidt condensation of 3-(1,2,3,6-tetrahydro-1-methylpyridin-4-yl)-2,4,5-trimethoxybenzaldehyde and various aromatic, heterocyclic and alicyclic amides of 3- aminoacetophenone afforded novel curcumin mimics. All the synthesized compounds were characterized by IR, ^{1}H NMR, Mass spectroscopy and evaluated for antioxidant, cytotoxicity and antimicrobial activity.



Curcumin



R= Aliphatic, Aromatic, Heteroaromatic

Assymetrical Curcumin mimics

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PP 17

REMOVAL OF BASIC DYE FROM AQUEOUS SOLUTION USING ECO FRIENDLY ADSORBENT

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The most concerned environmental pollutions are air pollution and wastewater pollution. Wastewater pollution comes from the industrial effluent and also from the domestic sewage etc. A large number of pollutants get mixed in the water; the processing wastewater contains many hazardous materials. Water pollution arises from the discharge of industrial and human wastes into freshwaters, estuaries, and oceans. This may result in the depletion of oxygen owing to excessive growth of microorganisms, which makes less of the water habitable for fish and other aquatic animals. Millions of tones of industrial and mining wastes, such as flash, blast furnace slag, phosphogypsum, red mud and mine tailings from different metals are discharged annually in our country. Industrial processes that feature physical and chemical changes have traditionally been designed without much thought to process waste and adverse environmental impacts of emissions and discharges. Dyes are found in wastewater streams of industrial processes including textile, rubber, pulp, paper, cosmetics, pharmaceutical, electroplating, food tanneries, leather, dye manufacturing, printing carpet, ceramics, surface treatment, pesticides, chemical fertilizers, municipal sewage, painting, coating, mining, extractive metallurgy, nuclear and other industries. Their removal has attracted much practical and academic interest owing to increased concern with their environmental impact.

Various physicochemical and biological methods have been studied for the toxic chemicals removal from industrial wastewater such as chemical precipitation, ion exchange, electrochemical reduction, exploration, ultra filtration phytoextraction, solvent extraction, membrane processes, filtration, flocculation, coagulation, complexation, sequestration, Chelating ion exchangers, cloud point extraction, flotation, sedimentation adsorption, etc. Most of these methods suffer with high capital and regeneration costs of the materials; drawback of chemical treatments is production of secondary pollutants due to excessive utilization of chemicals. Among the physiochemical processes, adsorption technology is considered to be more promising technique due to its efficiency, less cost, capacity and capability to eliminate dyes from industrial effluents on a large scale, the adsorption process is one of the effective methods for removal dyes from the waste effluent.

This study investigated the adsorption of a dye, namely Methylene Blue (MB), onto potato husk sample. The results shown that potatoes husk powder a relatively high adsorption capacity for MB. This adsorption is described by isotherms and thermodynamic parameters. This method has an advantage, as it can be applied in developing countries due to the low cost.

PP 18

MICROWAVE ASSISTED SYNTHESIS OF FLOUROCHLORO BENZIMIDAZOLO SUBSTITUTED THIAZOLIDINONE DERIVATIVES FOR ANTIMICROBIAL ACTIVITIES

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Benzimidazole is an antiprotozoal agent, was found as anthelmintics by Gregory in 1992, also used as anticancer agent by inhibiting Poly (ADP-ribose) Polymerase (PARP). To synthesize some novel flourochloro Benzimidazolo substituted thiazolidinone derivatives by establishing microwave assisted methods for synthesis of the proposed derivatives and confirm the various structures by spectral and elemental analysis. Evaluation of synthesized derivatives for their Biological activity is done. Further the Benzimidazolo-thiazolidinone derivatives have been reported for antimicrobial activity with one gram positive and one gram negative staphylococcus aureus and E coli agents. Thiazolidinone derivatives have been used as antidiabetic agent in view of the above and in continuation of search we have prepared benzimidazolo-thiazolidinon derivatives**.**

We have prepared flourochloro Benzimidazolo substituted thiazolidinone derivatives by reacting 3-chloro 4-flouro o-phenylenediamine with para amino benzoic acid and the aspartic acid respectively followed by different aldehyde and thioglycolic acid in presence of aluminium chloride. In future it is tested for anti-diabetic activity. A series of 12 derivative has been reported as antimicrobial agents with g(+ve) and g(-ve) bacteria.Derivatives are confirmed by TLC, Melting point, IR, NMR, Mass spectrometry. In antimicrobial activity it is seen to show better activity in gram negative bacteria E coli, and also it shows good activity in gram positive bacteria also.

PP 19

APPLICATIONS OF NATURAL CATALYSTS IN ORGANIC TRANSFORMATION: AS GREEN APPROACH

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The growing concern for the environment demands the development of environmentally benign and economic processes in organic syntheses, wherein even less hazardous byproducts are not desirable. In the development of new methodologies, ecological points of view must also be taken into account. Hence, development of non-hazardous synthetic methodologies for organic synthesis is one of the latest challenges to the organic chemists.

In accordance with this view, we are reporting the number of reactions for C-C and C-N bond formation by lemon juice as Natural catalyst. The catalyst is employed for reactions like Knoevenagel condensation between active methylene compound with aromatic aldehydes, Biginelli reaction as multicomponent reaction for the formation of dihydropyrimidines, for imine formation etc. without employing any organic solvent.

A number of improved procedures have been reported for these reactions. Some green methods have been reported by using catalyst and in the absence of solvent. However, these methods have various drawbacks such as high reaction temperature, prolonged reaction time, toxicity, low recovery and use of expensive catalysts. Therefore, introduction of clean procedures and utilizing eco-friendly green catalyst have attracted attention of workers. This catalyst yields the products in good quantity as compared with the other catalysts employed for these reactions.

In this work, we are reporting green approach for organic transformation using a catalytic amount of lemon juice at ambient temperature. In addition to its simplicity, this catalyst resulted in moderate to higher yields for the synthesized products. Further more the work up procedure were very simple and user friendly.

PP 20

SYNTHESIS AND BIOLOGICAL EVALUATION OF A NOVEL SERIES OF METHOXYLATED CHALCONES AS ANTIOXIDANT AND ANTI-MICROBIAL AGENTS

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A series of novel 2, 4, 5-trimethoxy Chalcones derivatives of biological interest were prepared by Claisen–Schmidt Condensation reaction. All the new compounds were evaluated for (1a-u) antioxidant (DPPH free radical scavenging activity) and antimicrobial (antifungal and antibacterial) activities against some selected pathogenic bacteria and fungi. Amongst all the 21 compounds screened, compounds 1b and 1o exhibited promising antioxidant activity (68 and 71% inhibition, as against standard BHA, 72 % inhibition) while compounds 1c, 1d, 1j and 1k exhibited antibacterial and compounds 1c, 1j and 1k exhibited promising antifungal activity (MIC of 10-30 µg/ml). The structure–activity relationship (SAR) for all the above stated activities has also been represented.

PP 21

DEVELOPMENT OF COMFA MODEL FOR AZD4877 ANALOGUES AS KINESIN SPINDLE PROTEIN (KSP) INHIBITOR

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AZD4877 emerged as research molecule of AstraZeneca (R&D Boston) and due to favorable pharmacokinetic profile and notable in vivo efficacy supported the selection of this compound as a clinical candidate for the treatment of cancer. In present investigation we are reporting the influence of different physicochemical and structural parameters on Kinesin spindle protein (KSP) inhibitory activity using comparative molecular field analysis (CoMFA). CoMFA model was generated by using Sybyl-X molecular modeling package. The data set of IC_{50} value related to antitumour activity was collected from literature (Maria-Elena Theoclitou *et. al.*). The most active compound AZD4877 (IC_{50} 0.002µm) in the present series was selected for alignment. After the generation of CoMFA, the statistical validity of the models was judged by high values of cross-validated q^2 (0.43) and non-validated r^2 (0.92), and also the lowest standard errors of estimation (SEE). The models that fulfill these criteria were selected for discussion. In SYBYL-X 1.1 settings, steric interactions are represented by green and yellow colored contours while electrostatic interactions are displayed as red and blue contours. The present CoMFA model nicely explains difference in the activity of the most active AZD4877 and other analogues.

PP 22

IRON-CATALYZED N-ARYLATION OF PHENYLUREA WITH ARYL HALIDES

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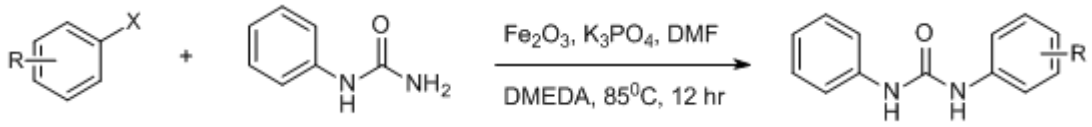
Transition metal catalyzed cross-coupling of aryl halides and amines provides an invaluable entry towards the synthesis of a wide range of compounds, including pharmaceuticals and natural products. *N, N'*-Diarylureas are valuable subunits for organic synthesis and have found numerous applications as drugs, pesticides, [1] selective anion-binding receptors [2] and polymer materials. The palladium catalyzed reactions are very sensitive to functional groups such as –OH, $–NH_2$, exogenous air or moisture and also very expensive compared to the copper reagent.[3] Kotecki has reported the palladium catalyzed amidation of urea with different aryl halides and Bippyphos was found to be a suitable ligand for these coupling reactions. [4] However, this method suffers from the following disadvantages: (1) the use of toxic phosphine ligands, (2) the palladium catalyst is expensive.

To develop economical and environment friendly routes in organic transformation we have tried the coupling reaction of phenylurea with different functionalized aryl halides in the presence of air stable Fe_2O_3, N, N-dimethylethylenediamine as a ligand, and K_3PO_4 as a base gives symmetrical and unsymmetrical diarylureas in relatively high yields. This method is milder than the palladium catalyzed arylation and avoids the use of toxic phosphine ligand. Present methodology deals with remarkable features like mild reaction condition, high yielding, shorter reaction time, easy workup and more importantly environmentally benign. We believe that this is an excellent complement to the previously established palladium- and copper-catalyzed *N*-arylation protocols.

Scheme:



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PP 23

RAPID ONE-POT, FOUR COMPONENT SYNTHESIS OF PYRANOPYRAZOLES USING HETEROPOLYACID UNDER SOLVENT-FREE CONDITION

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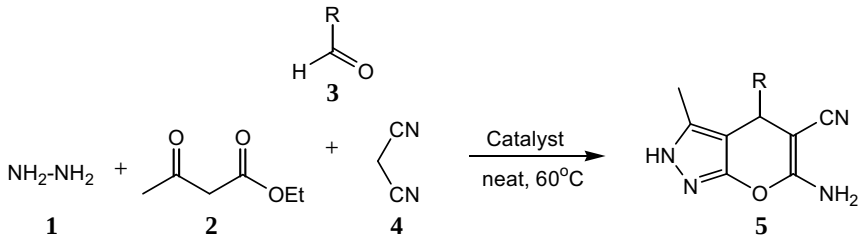
Pyranopyrazoles are an important class of biologically active heterocycles. They are reported to possess a multiplicity of pharmacological properties including anticancer, antimicrobial, antiinflammatory, insecticidal, and molluscicidal activities [1]. They are also potential inhibitors of human Chk1 kinase [2]. They also find applications as pharmaceutical ingredients and biodegradable agrochemicals. In a view of great importance of pyranopyrazoles, we report herein a simple, rapid and high yielding one pot four-component reaction protocol for the synthesis of pyranopyrazole derivatives employing environmentally friendly silicotungstic acid ($H_4[SiW_{12}O_{40}]$) as a catalyst under solvent free condition.



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PP 24

SYNTHESIS OF SOME NOVEL INDOLE DERIVATIVES USING DEXOYBENZOINS AS INTERMEDIATES

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Indoles exhibit anticancer, antiviral, antibacterial, antioxidant, cytotoxic and insecticidal activities. The indole moiety is present in a number of drugs currently present in the market. Most of these belong to "triptans" which are used mainly in the treatment of migraine headaches. All members of this group are agonists of migraine associated 5-HT_{1B} and 5-HT_{1D} serotonin receptors [1]. Sumatriptan (Imitrex) was developed by Glaxo for the treatment of migraines and introduced into the market as the first member of the triptan family [2].

The indoles **(4BPP001)** were synthesized from dexoybenzoins and substituted aryl hydrazines[3,4]. The compound **4BPP001** was reacted with methyl iodide under K_2CO_3/DMF condition and NH_4Cl under Py-BOP/HOBT/TEA to give alkylated **(4BPP002)** and amide **(4BPP003)** derivatives respectively. Aryl boronic acids were treated under Suzuki condition (Pd_2dba_3, X-phos, Na_2CO_3, ACN: H_2O) in microwave to afford various Suzuki coupled products **4BPP004-4BPP024**. Finally, free acid group of **4BPP001** reacted with different amines in presence of EDC.HCl, HOBT in basic medium to afford acid amine coupled products **4BPP025-4BPP029**.

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PP 25

COPPER (I) CATALYSED COUPLING OF QUINOLINE CARBOXAMIDE WITH STYRYL HALIDE: SYNTHESIS AND BIOLOGICAL EVALUATION OF PERSPICAMIDE ANALOGUES AS ANTILEISHMANIAL AGENT

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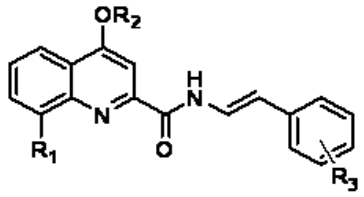
Natural product synthesis is highly demanding and most fascinating part of organic chemistry. Among which privileged structure Quinoline based natural products have shown broad range of biological activities. (1)In search of this, the metabolite perspicamide A & B having quinoline core nucleus along with secondary enamide sidechain, were first isolated from the Australian ascidian *Botrylloides persipicuum* Herdman 1886 (Styelidae) in 2005 by Matthew J. McKay etal(2). Enamides are important structural motif present in a large number of functionalized molecules with a wide variety of uses, including applications in medicinal chemistry, materials science, and several reaction intermediates. Enamide natural products salicylihalamide A and B, lobatmide A-F, apicularen A, Oximidines I and II , TMC-95A-D are already proven for their cytoxic activity & Isoechinulin-type alkaloids, IsoechinulinA, and Variecolorin C having radical scavenging activity, ultraviolet-A protecting activity, immunosuppressive activity, and antibacterial activity.(3). Among the emerging methods, for the synthesis of C-N bond formation, metal catalysed reactions found their application in the synthesis of biologically active natural products, particularly copper catalyzed reactions. Copper catalysts have significant role, because it is very cheap, non-toxic & mostly efficient in catalytic amount. Copper-catalyzed coupling reaction of amides with vinyl halides has received increasing attention because they highly enantioselective have functional tolerance and equally effective in prior as well as at a late stage in the synthesis.(4) Since long time our interest to synthesized quinoline based molecules as antiinfective activity. We report the first synthesis towards Perspicamide analogues, which were tested for their bioactivity (5) and few synthesised compounds showed moderate to good Antileishmanial activity.



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PP 26

TOTAL SYNTHESIS OF A TRIHYDROXYACID OXYLIPIN AND DETERMINATION OF ITS ABSOLUTE CONFIGURATION

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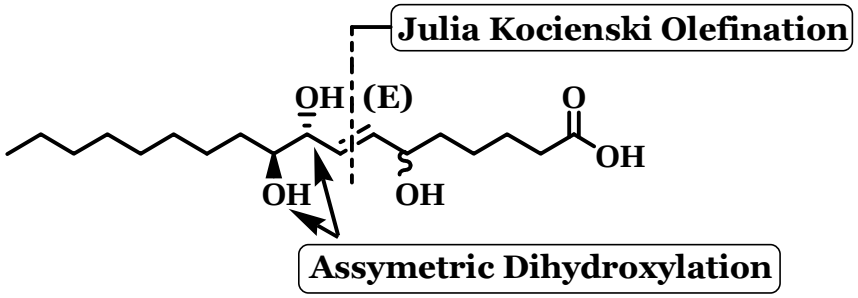
Total synthesis is an essential practice in organic chemistry in order to fulfill the growing demand of biologically important natural products. In the course of achieving complex synthetic targets, total synthesis serves as a powerful tool which demand discovery of new reagents, reactions and strategies. Oxylipin (9R, 10S, 7E)-6,9,10-trihydroxyoctadec-7-dienoic acid (**1**) was isolated from the n-butanol extract of the corms of *Dracontium loretense* (Benavides et al. [1]). The infusion obtained from the corms of *Dracontium loretense* has been traditionally used in Peruvian folk medicine to enhance immune function. In particular, together with the extract or infusion from *Uncaria tomentosa*, it is used by AIDS patients to reinforce the immune system. Oxylipin **1** exhibited an immunostimulatory effect on human peripheral blood mononuclear cell (PBMC) proliferation. In the context of our ongoing programme on the synthesis of pharmacologically important natural products (Saikia et al. [2]), we have developed a novel synthetic sequence of Oxylipin **1**. The details of the synthesis will be presented.



1

(9R, 10S, 7E)-6,9,10-trihydroxy-octadec-7-enoic acid (Trihydroxyacid Oxylipin)

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PP 27

CHROMATOGRAPHIC SEPARATION OF QUATERNARY MIXTURE OF PROCHLORPERAZINE MALEATE, ERGOTAMINE TARTARATE, PARACETAMOL AND CAFFEINE IN TABLET DOSAGE FORM BY REVERSED PHASE CHROMATOGRAPHY USING ION PAIRING REAGENT

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A Rapid reverse phase partion chromatography was developed using ion pairing reagents, for the simultaneous determination of Prochlorperazine maleate (PCM), Ergotamine Tartarate (EGT), Paracetamol (PCL) and Cafffeine (CFN) in pharmaceutical formulation. No single method was reported for the simultaneous estimation of all four components. Initial method development is started with the basic mobile phase pH 7.5. Several gradient programs have been tried but the PCM peak shape is not proper, so switched to acidic mobile phase. As the basic polar compound was protonated in acidic pH and eluted more quickly, also by keeping the pH of the mobile phase on the acidic side, the silanol interaction with basic analyte was minimized and peak symmetry and sensitivity of all analytes was improved. The separation of the all four components was performed on Purospher star RP-18e (150 x 4.6) mm 5µm column. Gradient program was used for the separation of all the components. Mobile phase A is water containing 0.4% Octane sulphonic acid sodium salt : glacial acetic acid (100:0.4) v/v and Mobile phase B is Acetonitrile. Method was linear giving correlation coefficient r^2 =0.9999 for PCM, r^2 =1.0000 for EGT, CFN and PCL.

PP 28

CONVENIENT AND EFFICIENT SYNTHESIS OF CHALCONES USING MOTMORILLONITE K-10 AS A CATALYST

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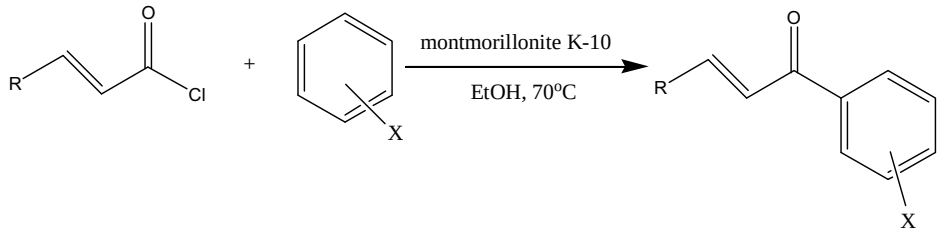
Chalcones, or 1,3-diaryl-2-propen-1-ones, belonging to the flavonoid family are one of the major classes of natural products with widespread distribution in fruits, vegetables, spices, tea and soy based foodstuff. They have been reported to possess diverse pharmacological activities including anti-cancer, anti-inflammatory, antimitotic, anti-tubercular, cardiovascular, cell differentiation inducing, nitric oxide regulation modulatory, and anti-hyperglycemic. They are also important due to their use as starting materials in the synthesis of series of heterocyclic compounds. Because of biological importance of chalcones, various methods have been described in literature. Herein we report montmorillonite K-10 catalyzed synthesis of chalcones at 70^{o}C in ethanol. Activated as well as unactivated aromatics smoothly underwent Friedel-Crafts acylation with α, β-unsaturated acid chlorides furnishing excellent yields of the corresponding chalcones.



PP 29

METAL-LIGAND EQUILIBRIA IN SOLUTION: A PERSPECTIVES OF BIOLOGICALLY IMPORTANT COMPOUNDS

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Chelation enables metals to be transported to or from vulnerable target sites, and to hinder or facilitate their carcinogenic potential. In the reverse sense, metals are capable of ligand scavenging via complexation; metal complexes can be utilized for the transport of selected organic chemotherapeutic drugs to target organs, or for the decorporation of those toxic organic compounds which are able, before or after metabolic activation, of reacting with metal complexes. The transition metal ions inevitably exist as metal complexes in biological systems by interaction with the numerous molecules possessing grouping capable of complexation or chelation. Hence we find essential metals such as Cu, Zn, Co etc. existing as binary and ternary chelates of amino acids, carboxylic acids, and proteins. Without such interactions, life could not exist or be maintained, or, as earlier expressed; life could not exist or even come into being without the mediating action of metals. Metals are involved in every aspect of biosynthesis, biodegradation, and in the assembly of macromolecular structure. The biochemistry is the coordination chemistry of organic chemistry and metal ions of living systems. Metals are involved in such a large number of essential biological reactions that life as we know it could not exist without coordination compounds. Keeping in view, the above fact, We studied the stability constants of some complexes of transition metal with biological ligands such as Ciprofloxacin.HCl, Ascorbic acid, Pyridoxine.HCl. The study reveals that the order of stability of above complexes is in the following order M-Ascorbic acid> M-Pyridoxine.HCl> M-Ciprofloxacin.HCl.

PP 30

SPECTRAL,THERMAL AND FUNGICIDAL STUDIES OF SCHIFF BASE METAL COMPLEXES DERIVED FROM 3-ACETYL-6-METHYL-(2H)-PYRAN-2,4(3H) DIONE.

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The solid complexes of Cu(II), Ni(II), Co(II), Mn(II) and Fe(III) with Schiff base ligands derived from heterocyclic compounds 3-acetyl-6-methyl-(2H)-pyran-2,4(3H)dione (Dehydroacetic acid) and o-chloroaniline were synthesized and characterized by elemental analysis, conductance, magnetic, thermal, uv-vis and ^{1}H-NMR spectroscopy. The ligand field parameters have been evaluated for Cu(II), Ni(II), Co(II), Mn(II) and Fe(III) complexes which suggest an octahedral geometry for each of them. The magnetic moment and spectral data suggest the dimeric nature of Mn(II) complexes with octahedral geometry. The fungicidal activities of the ligands and their metal complexes have been screened in *vitro* against *Aspergillus niger* and the percentage inhibition of the metal complexes is found to be increased considerably then that of their corresponding ligands and the order is Cu>Ni>Fe>Mn>Co.

PP 31

ORGANIC TRANSFORMATIONS IN AQUEOUS MEDIA: IN-SITU GENERATED HCL CATALYZED SYNTHESIS OF 14*H*-DIBENZO[*A*, *J*]XANTHENES

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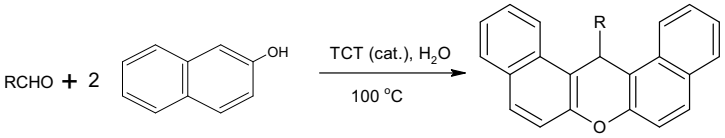
Xanthenes and particularly benzoxanthenes derivatives are biologically important nitrogen heterocycles due to their antiviral, antibacterial and anti-inflammatory activities Lambert et al [1]. Benzoxanthene derivative have also shown promising activity as sensitizer in photodynamic therapy as well as controlling localized tumers Poupelin et al [2]. There are many reports on the synthesis of xanthene derivatives including aryne cycloaddition to phenols, intramolecular coupling of aldehydes and ketones, cyclodehydration, the reaction of β-naphthol with formamide, α-naphthol-1-methanol and carbon monoxide Hamid et al [2]. Recently, these compounds have been prepared by mixing β-naphthol with aldehydes in the presence of various catalysts such as Amberlyst-15, LiBr, sulfamic acid, p-TSA and I_2 Sandhu et al [3]. These methods have one or other disadvantages such as drastic reaction conditions, very long reaction times, need of special apparatus and the use of hazardous solvent.

In the present work, we report an efficient one-pot condensation of β-naphthol with aldehydes in presence of cyanuric chloride under aqueous medium for the synthesis of 14-substitued-14-*H*-dibenzo[*a*, *j*]xanthenes.



The advantages of the present protocol are: (i) use of inexpensive catalyst (ii) use of water as a green solvent (iii) method works well on 100 mmol scale therefore, applicable on large scale synthesis of these derivatives and (iv) purification of the product using column chromatography is not required.

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PP 32

DEVELOPMENT OF A LC-MS METHOD FOR THE DETERMINATION OF DEGRADATION IMPURITIES OF DULOXETINE HYDROCHLORIDE IN ORAL SOLUTION

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Duloxetine HCl, (+)-(S)-N-Methyl-3-(naphthalen-1-yloxy)-3-(thiophen-2-yl)propan-1-amine hydrochloride is a selective serotonin and norepinephrine reuptake inhibitor and it has been approved for the treatment of major depressive disorder and for the management of diabetic peripheral neuropathic pain.

The thorough literature survey reveals that, there are some HPLC methods are reported for the assay, related substances and chiral purity of Duloxetine. Besides the reported impurities, we have observed three potential impurities i.e. two were increasing in accelerated stability condition and one was increasing in sample solution stability. So we developed a LC-MS method which will be helpful for probable elucidation of structure of unknown impurities.

The chromatographic separation was achieved on Grace Kromasil C18, 250 mm X 4.6 mm, 5 µm column using a mobile phase system consisting of 0.5 ml per litre of trifloroacetic acid per litre as mobile phase A and acetonitrile as mobile phase B with gradient elution. The mobile phase was pumped on the column at the flow rate of 1.5 mL min-1. Column oven temperature used was 40°C. The detector wavelength selected was 230 nm. The developed LC-MS method shows sensitivity and selectivity. Mass spectral data add specificity that increases confidence in the results of both qualitative and quantitative analysis.

PP 33

COMBINATORIAL SYNERGISTIC EFFECT OF MARIZOMIB AND VORINOSTAT IN CANCER

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Combining proteasome and histone deacetylase (HDAC) inhibition has been noticed to provide synergistic anti-tumor activity, with complementary effects on a number of signaling pathways. Marizomib is an orally active, nonpeptide small molecule proteasome inhibitor that induces apoptosis in multiple myeloma and leukemia cell lines and patient cells as well. Vorinostat (SAHA) is a histone deacetylase inhibitor that modulates the transcription of multiple genes including those affecting cell-cycle and apoptosis in cancer cells. In our *in vitro* studies we evaluated the possible efficacy of combining marizomib and vorinostat. Combinations of marizomib and vorinostat were assessed *in vitro*. Combination index (CI) values of marizomib and vorinostat were calculated to see whether these combinations have synergistic, additive or antagonistic effect. Treatment of NSCLC tumor cell lines with marizomib and vorinostat resulted in a highly synergistic antitumor activity. Our results demonstrate that synergistic (CI<1) growth inhibitory effects could be seen in all the eight lung cell lines studied. Conspicuous synergy of marizomib and vorinostat was observed in tumor cell lines derived from patients with NSCLC carcinoma. Further details will be revealed during the presentation.

PP 34

4-AMINOQUINOLINE BASED SCAFFOLDS AS POTENTIAL ANTIMALARIAL AGENTS

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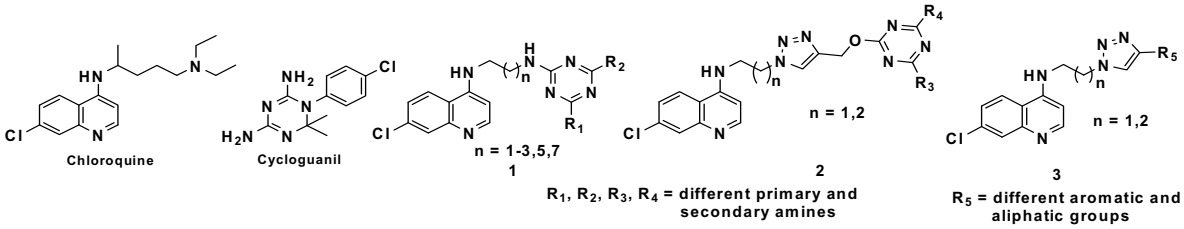
Malaria is the third most infectious disease after HIV and tuberculosis in terms of human suffering. World Health Organization (WHO) estimation shows that about 225 million cases of malaria occur annually with 0.7-1.0 million deaths a year and about 50% of world population is at risk of suffering from malaria [1]. It has been found that among the four *Plasmodium* species that causes malaria, *P. falciparum* is the most virulent and accounts for most of the malaria related deaths [2]. Global diffusion of drug-resistant strains of *P. falciparum* to many of the existing antiamalarials such as chloroquine and others has brought a serious setback in efforts for combating malaria. Despite this, 4-aminoquinoline class of therapeutics, to which chloroquine belongs, remains a frontline drug of choice based on its excellent clinical efficacy, ease of administration, low toxicity and cheap synthesis [3]. It has been found that modification of the basic side chain of chloroquine by linking it with other antimalarial scaffolds such as triazines can lead to improved hybrid antimalarials active against drug resistant *P. falciparum* strains [4].



Keeping these points in mind, and as a part of our ongoing research on malaria [5-8], we have synthesized a series of 4-aminoquinoline-triazine (**1**) and 4-aminoquinoline-triazole (**2** and **3**) conjugates and evaluated their antimalarial activity against D6 (chloroquine-sensitive) and W2 (chloroquine-resistant) strains of *Plasmodium falciparum.* Some of the tested compounds have shown potent antimalarial activity compared to chloroquine [9, 10].

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PP 35

DESIGNING OF CHIRAL CATALYST FOR ASYMMETRIC CYANATION REACTION

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Chiral cyanohydrins and iminonitriles are versatile building blocks for pharmaceuticals, agrochemicals and specialty materials. A number of efficient and successful synthetic methods have been developed however, the chiral catalytic method is one of the most attractive strategies where asymmetric addition of different source of cyanide to the carbonyl group of aldehydes ,ketones and imines was affected with the help of a chiral metal complex. I will discuss the various methods for catalytic asymmetric synthesis of cyanohydrins and iminonitrile derived from both aldehydes, ketones and imines using different source of cyanide. The emphasis would be given to chiral Lewis acid metal complexes as well as organo-catalyst.

PP 36

A GREEN AND HIGHLY EFFICIENT SYNTHESIS OF THIOETHERS UNDER SOLVENT-FREE CONDITIONS AT ROOM TEMPERATURE

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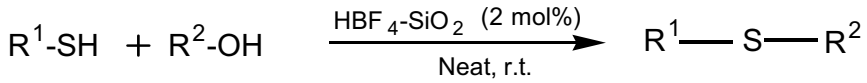
Thioethers have emerged as a prominent class of organic compounds; they have useful applications as key reagents in organic synthesis, in agro-chemicals, and in bioorganic, medicinal, and heterocyclic chemistry. Thioether linkage has been used to prepare cyclic analogues of acyclic polypeptides to restrict their conformation mobility and thus to increase their biological activity and stability against biodegradation.

Some of the most common approaches to the synthesis of thioethers are the Salkylation of thiols under the conditions of Mitsunobo reaction, by the deoxygenation of sulphoxides, the displacement of leaving groups with sulphur nucleophile, the addition of thiols to carbonyl compounds followed by the in-situ reduction of the generated intermediate thionium ion, an anti-Markonikovaddition of arenas and alkanethiols to alkenes, the metal mediated cross-coupling processes or the metal-catalyzed hydrothiolation of alkynes.



In this communication we report the $HClO_4$-SiO_2 catalyzed efficient and convenient synthesis of thioethers from various alcohols with thiols in high yields under solvent-free conditions at room temperature. In our process, when the catalytic reaction was completed, $HClO_4$-SiO_2 could be recovered conveniently from the reaction mixture and used further for the next cycle without activation, only through filtration and subsequent washing with ethyl acetate.

PP 37

SYNTHESIS OF NOVEL *E*-CINNAMAMIDES CONTAINING HETEROCYCLIC RING STRUCTURE

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Hetero atoms in the structure may change the activity of molecule which increases its applications in different fields(1-6). Considering this simple fact of heteroatom (7-10) a series of cinnamamides containing heterocyclic ring were synthesized and the compounds were screened for their biological activities. The synthesized compounds shows interesting biological activities against selected pathogens. These compounds may be use in medicinal field for variety of applications (11). Structures of the compounds were confirmed by spectroscopic techniques.

Key words: Heteroatom, Cinnamamides

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PP 38

A CONVENIENT SYNTHESIS OF A NOVEL CLASS OF A/B-RING FUSED STEROIDAL TETRAZOLES

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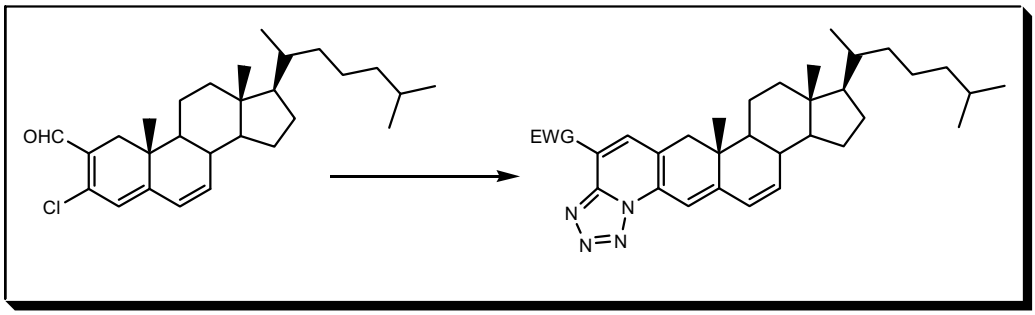
The steroidal heterocycles constitute one of the most interesting classes of organic compounds and their biological activities are well documented.[1] Tetrazoles and their derivatives are present in many of the bioactive heterocyclic compounds that are reported to possess wide range of pharmacological applications such as antibacterial, antifungal, antiviral, analgesic, anti-inflammatory, antiulcer activities.[2] Tetrazoles are considered to be isostere of carboxylic acid group and they are therefore, extensively studied for their biological importances.[3] Only few examples are there in literature citing synthesis of steroidal tetrazoles[4,5] using excess of hydrazoic acid. Thus, in continuation of our studies on the synthesis of azasteroids, [6] herein we report our results on synthesis of some novel A/B ring fused steroidal tetrazoles using chloroformyl system via azide-nitrile cycloaddition reactions.



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PP 39

SYNTHESIS AND BIOLOGICAL EVALUATION OF BISTRIAZINE AS A POTENTIAL ANTILEISHMANIAL AGENT

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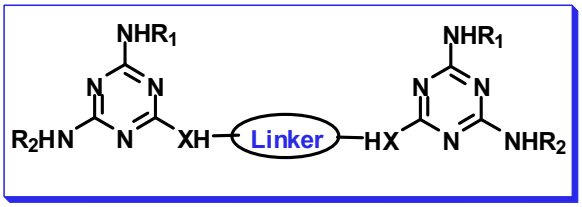
Leishmaniasis is endemic in >85 developing countries with >1.5 million estimated cases occurring each year and an additional 350 million people at risk of infection. Leishmaniasis is vector-borne disease caused by blood and tissue dwelling protozoan parasite species belonging to the genus Leishmania.1 It is the second-largest parasitic killer of humankind with its three clinical forms; Cutaneous Leishmaniasis and Mucocutaneous Leishmaniasis, which are less severe form of the disease with usually self-healing ulcers.2 Due to development of resistance against pentavalent antimonial compounds in India to such an extent that they can no longer be used in some regions. Only recently amphotericin B, pentamidine, and miltefosin have been discovered as effective antileishmanial drugs. All these drugs suffer also from serious side effects associated with them.3 Thus, there is a clear need for development of less toxic drugs based on new molecular scaffold that are effective against all forms of leishmaniases.

Dihydrofolate reductase (DHFR) has successfully been used as a drug target in the area of parasitic diseases. But most of the clinically used DHFR inhibitors show less selectivity for leishmanial enzymes.4 Triazine class of compounds being the inhibitors of DHFR has also been identified as potential antileishmanial agents.5 Based on these observations we have designed and synthesized the bis-triazines joined with the help of linker. These compounds were screened for their antileishmanial profile and have shown encouraging results against *Leishmania donovani*.



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PP 40

CYANURIC CHLORIDE CATALYZED MILD PROTOCOL FOR SYNTHESIS OF BIOLOGICALLY ACTIVE DIHYDRO/SPIRO QUINAZOLINONES AND QUINAZOLINONE-GLYCOCONJUGATES

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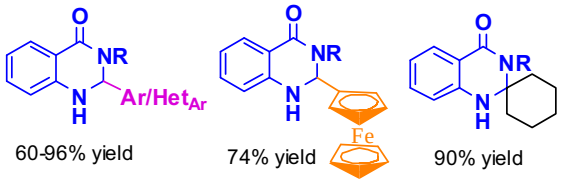
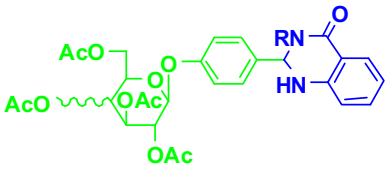
In the community of fused heterocycles, 2,3-dihydroquinazolin-4(1*H*)-one and 2-spiroquinazolinone are omnipresent and have been referred to as "core structures" in drug discovery. These quinazolinones displayed wide range of biological activities as antitumor [1], antidefibrillatory [2], antidepressant [3], analgesic [4], etc. On the other hand corresponding quinazolin-4(3*H*)-one are also important building blocks in natural products (Rutaecarpine) [5] and the compounds of pharmacological interest [6].

Earlier methods for synthesis of these molecules have limited scope. Therefore, here we developed an efficient cyanuric chloride catalyzed approach for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-one, 2-spiroquinazolinone, spirooxyindole and glycoconjugates of 2,3-dihydroquinazolin-4(1*H*)-one derivatives. The reaction allows rapid cyclization (8-20 min) with 10 mol% TCT to give skeletal complexity in good to excellent yield.



60-96% yield 74% yield 90% yield



68-72% yield

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PP 41

SYNTHESIS AND ANTIDIABETIC ACTIVITY OF SOME NEW N^1-ARYL-N^3-[4'-2"-ARYL-4"-OXO-THIAZOLIDIN-3"-YL) BENZENE SULPHONYL]-THIOUREAS

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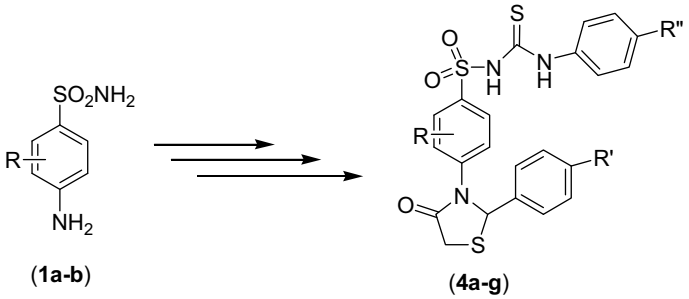
Diabetes mellitus is now recognized as a serious global health problem and has broken the age barrier. World health organization report asserts that India has the highest number of diabetes in the world. It is projected that by 2025, there will be 60-70 million diabetics in India.

Sulfonyl thioureas and 4-thiazolidinones constitute an important class of compounds in drug research due to their ability to stimulate the release of insulin from the pancreatic islets. Among the drugs available for the treatment of diabetes, 4-thiazolidinone derivatives are found to be more safer oral drugs, improving insulin sensitivity and lowering blood glucose, free fatty acids and triglycerides levels.

Considering the clinical efficacy of 4-thiazolidinediones and sulphonyl ureas, it was thought worthwhile to combine sulfonyl thioureas with 4-thiazolidinones in one molecular frame work, in order to obtain an effective lead molecules. Hence, in the present investigation, attempts have been made to synthesise the titled new sulphonyl thioureas, starting from sulphanilamides.

First the sulphonilamides(**1a-b**) have been condensed with aryl aldehydes and the obtained intermediates, 4-arylidenamino benzene sulphonamides (**2a-g**). The intermediates (**2a-g**) on subsequent cyclocondensation yielded 2-aryl-3(4'-sulphonamidophenyl)-4-thiazolidinones (**3a-g**). The condensation of aryl isothiocyanates and thiazolidinones (**3a-g**) was then carried for obtaining the titled products, N^1-aryl-N^3-[4'-2"-aryl-4"-oxo-thiazolidin-3"-yl) benzene sulphonyl]-thioureas (**4a-g**). The structures of all the synthesized compounds were established by analytical and spectral data. All the compounds have been evaluated for antidiabetic activity using alloxin induced rat models. The details of the synthetic path and the antidiabetic activity will be presented.



(**1a-b**) (**4a-g**)

PP 42

A NOVEL APPROACH FOR THE SYNTHESIS OF SOME A-RING ANNELATED STEROIDAL TRIAZOLE DERIVATIVES

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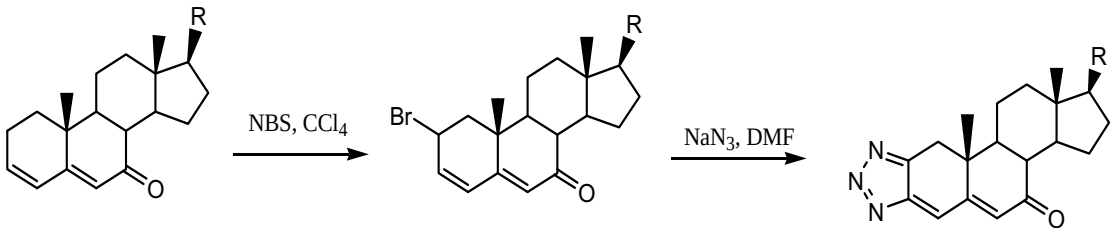
The steroidal heterocyclic compounds and their related systems have potential biological activity in the emerging field of antitumor drugs [1]. As for example, the A-ring annulated azasteroids such as danazole is well known drug against breast cancer and bone marrow cancer. Also, D-ring anneleted heterosteroids like 17-imidazolyl steroid is reported to exhibit excellent biological activities against prostate cancer [2]. The biological activities of heterosteroids may be accounted due to the heterocyclic ring fused to the steroidal moiety [3]. Attempts have been made to incorporate of heteroatom (N or O) in the steroidal molecule that can act as novel drug molecules with enhanced activities. The convenient synthesis of triazole via CuI/Et_3N catalyzed 'click chemistry' from azides are already reported [4]. In continuation of our studies [5], herein we report our results of synthesis of some steroidal triazole derivatives by substitution reaction of steroidal bromo derivatives followed by intramolecular cyclization of azido group.



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PP 43

Pd^0 CATALYZED REACTIONS OF CH_3HgI WITH ORGANIC HALIDES

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Among the transition metals, palladium has well established chemistry in (0), (II) and (IV) oxidation states and therefore it is widely used as a catalyst in organic synthesis [1, 2, 3]. Organomercurials are thermally stable compounds, they do not react with atmospheric oxygen and moisture, and can be synthesized by a number of synthetic routes and therefore it is of interest to use them in organic synthesis.

Pd^0 catalysed acyldemetallation reaction of CH_3HgI with acylhalide, in the presence of iodide ion as the nucleophilic catalyst, provide a mild and selective method for the synthesis of ketone (01). The catalytic cycle of the reaction involves a sequence of oxidative addition, transmetallation and reductive elimination steps.

$$ArCOCl + CH_3HgI \xrightarrow[\text{Acetone, 20-30 min.}]{Pd^0,\ I^-,\ \text{r. t.}} ArCOCH_3 \quad (70\text{-}80\%) \qquad (01)$$

Ar = C_6H_5, p-FC_6H_4, p-ClC_6H_4, p-BrC_6H_4 and p-$NO_2C_6H_4$

Catalyst: $PdCl_2(C_6H_5CN)_2$, $PdCl_2(PPh_3)_2$, $PdBr_2(PPh_3)_2$ and $Pd(OAc)_2(PPh_3)_2$.

I^-: NaI

Pd^0 catalysed carbonylation reaction of CH_3HgI with arylhalide, in the presence of iodide ion (a neucleophilic catalyst), provide another route for the synthesis of ketone (02). The catalytic cycle of the reaction involves a sequence of oxidative addition, insertion of carbon monoxide, transmetallation and reductive elimination steps.

$$ArI + CH_3HgI + CO \xrightarrow[\text{HMPA, 1.5 to 7 h.}]{Pd^0,\ I^-,\ \text{r. t.}} ArCOCH_3 \quad (70\text{-}75\%) \qquad (02)$$

(1 atm.)

Ar = C_6H_5 and p-$NO_2C_6H_4$

Catalyst: $PdCl_2(C_6H_5CN)_2$, $PdCl_2(PPh_3)_2$, $PdBr_2(PPh_3)_2$ and $Pd(OAc)_2(PPh_3)_2$

I^-: Bu_4NI

In the acyldemetallation and carbonylation reactions, Pd^0 is generated in the reaction mixture under reactions conditions from the initial palladium catalyst. The nucleophilic catalyst (iodide ion) plays an important role in acyldemetallation and carbonylation reactions. It forms an ionic complex $(Pd^0I)^-$ with Pd^0 and therefore precipitation of Pd-black is prohibited. Secondly it forms an ionic complex $(CH_3HgI_2)^-$ with CH_3HgI and hence fission of C-Hg bond becomes easier in transmetallation step. We conclude that Pd^0 and iodide ion catalysed acyldemetallation and carbonylation reactions of CH_3HgI with organic halides provide selective methods for the construction of new C-C bond.

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PP 44

AN EFFICIENT AND OPERATIONALLY SIMPLE SYNTHESIS OF SOME NEW N^1-SUBSTITUTED PYRAZOLE DERIVATIVES BY USING GRINDING TECHNIQUE

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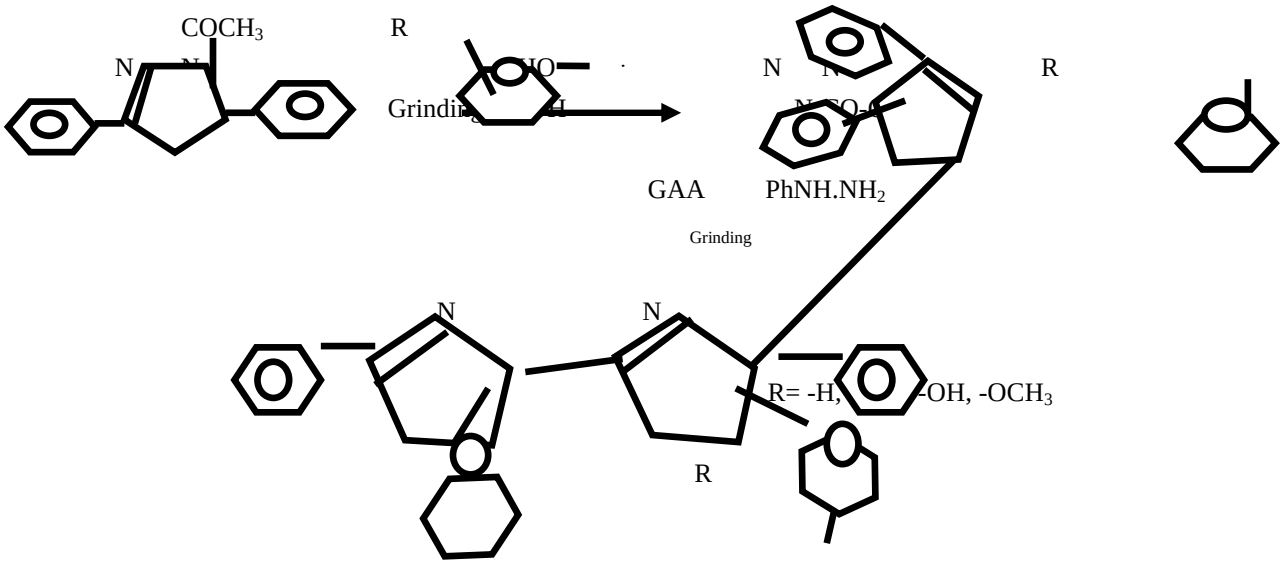
An efficient and operationally simple reaction between N-acetyl pyrazole with different aryl aldehydes gives corresponding chalcones followed by reaction with phenyl hydrazine in presence of glacial acetic acid afford N^1- (substituted) pyrazole derivatives by using grindstone with excellent yield and require short time period , mild reaction condition, environmentally safer and notable advantage of this method as per scheme.

SCHEME



PP 45

ONE-POT, THREE COMPONENT SYNTHESIS OF HIGHLY SUBSTITUTED PYRIDINES

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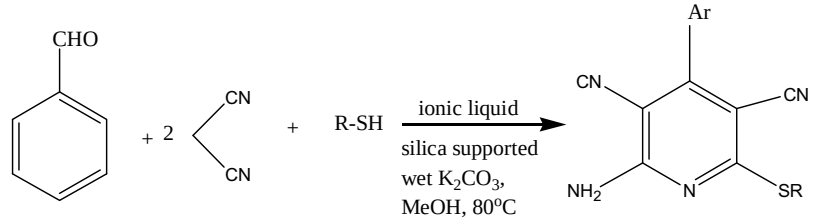
Pyridine nucleus is medicinally useful scaffold which occures in wild variety of both naturally and synthetic bioactive compounds. The highly substituted pyridine derivatives like 2-amino-4-aryl-3,5-dicyano-6-sulfonyl pyridines exhibit diverse pharmacological activities and are useful as anti-bacterial, anti-prior, anti-hepatitis B virus, anti-cancer agents and as potassium channel openres for the treatment of urinary incontinence.[6] In addition, many of these compounds are found to be highly selective ligands for adenosine receptors, which were recognised as potential targets for the development of new drugs for the treatment of Parkinson's disease, hypoxia/ischenia, asthma, kidney disease, epilesy and cancer. They are also imerged in potential medicinal used in developing therapeutic agents for the treatment of Creutzfeldt-Jacob disease.

Owing is their vast medicinal usefulness, various methods have been exployed for the preparation of substituted pyridine. Herein we report one-pot, three component synthesis of 2-amino-4-aryl-3,5-dicyano-6-sulfonyl pyridines from the reaction of aromatic aldehydes, malononitrile and thiophenol using ionic liquid in combination with wet silica supported K_2CO_3 in methanol at 80^{o}C as catalyst at room temperature is described.



Scheme-1

PP 46

ORGANIC ACID CATALYZED SYNTHESIS OF 2,3-DIHYDROQUINAZOLIN-4(1H)-ONES DERIVATIVES VIA MCR

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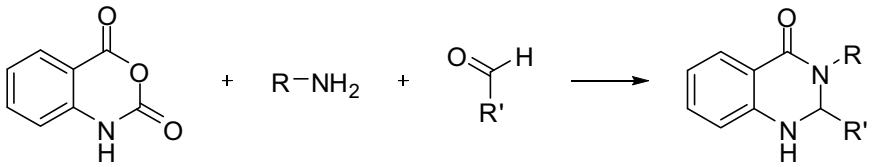
Environment friendly designing of efficient chemical process to minimize the use and generation of hazardous substances has become essential demand of modern organic synthesis. In this context, Atom economic multicomponent reactions (MCRs) have become a very appealing methodology since time, energy, labor, resources consuming workup and purification steps can be minimized in a synthetic sequence [1]. MCRs are at a premium for the achievement of high level of diversity in the synthesis of bio-active heterocyclic scaffolds. 2,3-dihydroquinazolinones, an important class of biologically active heterocyclic compounds, have been reported as antibiotic, antidefibril-latory, antispermatogenic, vasodilatory, and analgesic [2]. Moreover, these compounds can be further oxidized to their quinazolin-4(3H)-one analogues, an important class of biologically active heterocyclic compounds [3] that is also found in some natural products [4]. However, various improved methodology for the synthesis of 2,3-dihydroquinazolin-4(1H)-one have been reported in the literature [5] but many of these methods are not environmentally friendly and suffer from harsh reaction conditions. In the context of our interest in the synthesis of biologically important heterocycles via multi-component reactions, we have developed an efficient and organic acid catalysed MCR capable of affording a library of pharmacologically relevant 2,3-dihydroquinazolin-4(1H)-ones derivatives in good yields.



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PP 47

SPECTRAL, MAGNETIC AND THERMAL STUDIES OF NICKEL(II) COMPLEXES OF HETEROCYCLIC SCHIFF BASES

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Nickel(II) complexes of heterocyclic Schiff bases, derived from 4-(o-hydroxyphenyl) – 2-aminothiazole and R substituted salicylaldehyde (R=H, 3- Me, 4- Me, 5-Me , 5-Br, 5-Cl, 3-OMe) and 2-hydroxy-1-naphthaldehyde, have been synthesized and characterized by elemental and spectral (uv-vis and ir) analyses, conductivity and magnetic susceptibility measurements, and thermal studies. From the electronic spectra of the complexes, various ligand field energy parameters (Racah parameters B and C, nephelauxetic ratio β , Slater-Condon parameters F_2 and F_4, Slater-Condon-Shortley parameters F^2 and F^4 and h_X values) have been calculated. . A representative complex has been chosen for thermal studies. The complex undergoes decomposition in three stages (stage I: 225-395^{0}C, stage II: 395-495^{0}C, stage-III: 495-615^{0}C).The various kinetic parameters (n, E, Z, ΔS and G) have been calculated using Coats-Redfern, MacCallum-Tanner and Horowitz-Metzger methods.

Coats-Redfern Method

$$\left\{\log\left[\frac{1-(1-\alpha)^{1-n}}{(1-n)T^2}\right]\right\} = \log\frac{ZR}{Eq}\left[1-\frac{2RT}{E}\right] - \frac{E}{2.303R}\left(\frac{1}{T}\right) \qquad \ldots\ldots 1$$

MacCallum- Tanner Method

$$\log\left(\frac{1-(1-\alpha)^{1-n}}{(1-n)}\right) = \log\frac{ZE}{Rq} - 0.485E^{0.435} - \frac{0.449 + 0.217E}{T}\cdot 10^3 \qquad \ldots\ldots 2$$

Horowitz – Metzger Method

$$\log\left(\frac{1-(1-\alpha)^{1-n}}{(1-n)}\right) = \log\frac{ZRT_S^2}{Eq} - \frac{E}{2.303\,RT_s} + \frac{E\,\theta}{2.303\,RT_s^2} \qquad \ldots\ldots 3$$

(where α: fraction decomposed, q: heating rate,T: absolute temperature, Ts: temperature at half weight loss, n:order of reaction, Z: pre-exponential factor, E:energy of activation.)

The complexes are monomeric and non-electrolytic in nature and possess 1:2 metal:ligand stoichiometry. The uv-visible spectral data coupled with magnetic susceptibility values indicate that the complexes have an octahedral geometry. The values of nephelauxetic ratio β suggest that the complexes are covalent in nature. The h_X values indicate that the ligands (Schiff bases) should be placed in between urea and ammonia in the nephelauxetic series .The ir spectral studies show that coordination to the central metal atom takes place through nitrogen of the azomethine group, nitrogen of the thiazole moiety and oxygen of the phenolic OH group. The complexes are thermally stable and the values of kinetic parameters estimated by all three methods are in accordance with each other.

PP 48

NEW PATENT REGIME AND INDIAN PHARMACEUTICAL SECTOR.

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The Indian pharmaceutical industry is leading manufacture sector in India. After independence, the Indian Patent Act 1970 was framed which provided Process Patents for pharmaceuticals .As the monopoly rights in area of drugs were excluded from this act , the growth of Indian generic drug manufacturing industry was promoted resulting in to low cost of drugs. So far India was regarded as a supplier of low cost generic version of patented drugs to least developed countries. Today, the Indian Biotech market is dominated by Bio-pharmaceuticals (75%), mainly contributed by vaccines. Since 1995, the number of Biotech patents is increasing and the focus is on medical Biotech. In 2005, in compliance with World Trade Organisation's Trade Related Intellectual Property Rights (TRIPS), new Product Patent law (2005) which provides patent protection on both products and processes was implemented. This was a radical shift from Process Patent System to Product Patent System and the new Product Patent System does not allow marketing of generic drug, a drug patented elsewhere by using different processes. TRIPS implementation will eventually cut the life-time of affordable drugs, unless safeguard measures within the scope of TRIPS provisions to limit the rise in the prices of drugs are executed. Novartis's case for patent on Gleevece -an anti-cancer drug has implications for access to medicines at affordable price. Flexibilities available under TRIPS (Compulsory License) have to be utilised to protect public health. The Indian pharmaceutical companies can take benefit of rich biodiversity and focus on herbal products and alternative medicine products.

PP 49

CONCISE CONSTRUCTION OF INDOLE ALKALOIDS TYPE COMPOUNDS VIA BIFUNCTIONAL UGI-3CC FOLLOWED BY BICHLER-NAPLESKI REACTIONS

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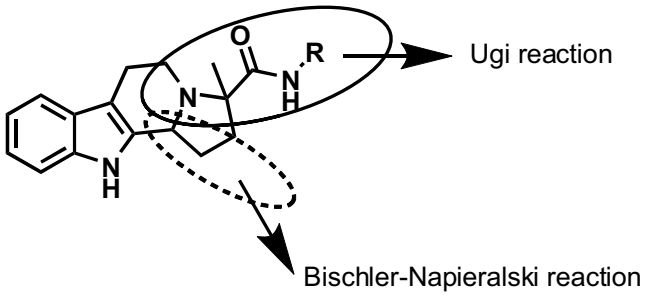
Indole alkaloids are the main group of bioactive alkaloids, including, for example, hypertensive reserpine, antiproliferative vinblastine, or antiprotozoal apicidin[1].The basic skeleton of indole alkaloids, however, is often only accessible via lengthy sequential synthesis. To optimize the properties of natural products or to efficiently discover novel unrelated biological activities, flexible synthetic approaches are in high demand. An efficient synthesis should lead into a target scaffold in a few synthetic steps, in good yields, and allowing for extensive variation of the different starting materials to broadly cover the respective chemical space. A stereoselective procedure should be possible as well. Multicomponent reaction (MCR) chemistry is a technique that allows for efficient and diverse access to multiple bioactive scaffolds [2].This technique recently led to multiple biological active compounds currently undergoing clinical evaluation or even being marketed [3]. As part of our ongoing program to identify new and efficient access to scaffolds of biological interest, we herein report a new and versatile MCR synthesis of Indole alkaloids (Figure).



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PP 50

SYNTHESIS OF DIVERSE 2,3-DIHYDROPYRAZINO[1,2-A]INDOLE-1,4-DIONE AND 2,3-DIHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE DERIVATIVES VIA TANDEM UGI-4CR / INTRAMOLECULAR CYCLIZATION

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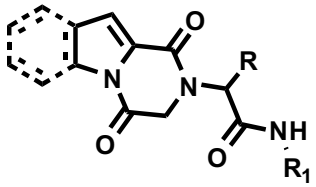
Heterocycles containing the 2,5 diketopiperazine scaffold are important targets in synthetic and medicinal chemistry because this fragment is present in a plethora of natural and synthetic biologically active agents. Various heteroaryl-fused 2,5 diketopiperazine fragments are present in a number of natural . Among them are Gliotoxin[1],WIN-64821[2], Spirotryprostatin A[3], Brevianamide[4], Demethoxyfumitremorgine C[5].

Herein we report an efficient approach for the synthesis of diverse 2,3-dihydropyrazino[1,2-a]indole-1,4-dione and 2,3-dihydropyrrolo[1,2-a]pyrazine-1,4-dione.The procedure combine the Ugi four-component reaction followed by the intramolecular cyclization of the Ugi product in one-pot procedure[6,7], which afford the desired products in good to excellent yields.



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PP 51

DESIGNING AND SYNTHESIS OF B-CARBOLINE-QUINAZOLINE HYBRID MOLECULES AS ANTILEISHMANIAL AGENTS

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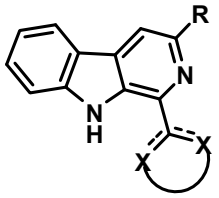
Leishmaniasis is a growing health problem in many parts of the world, with about 350 million people living in areas of disease endemicity and about 2 million new cases each year. Natural and synthetic β-carbolines and tetrahydro-β-carbolines alkaloids are well-known compounds that possess a variety of biological properties. In 1998, a tetrahydro-β-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*.[1] Later, annomontine, a pyrimidine-β-carboline alkaloid, isolated from the bark of a Brazilian tree *Annona foetida*,[2] was also reported to be active against leishmania.

Quinazoline is a significant pharmacophore of a number of natural products and have shown good biological activites.[3] Peganine hydrochloride has been identified as an active antileishmanial agent isolated during the bioassay guided fractionation on Peganum harmala seeds.[4] It has also been identified as trypanothione,[5] pteridine reductase 1[6] and DHFR[7] inhibitor responsible for its activity against leishmania. On the basis of above observations we designed a β-carboline-quinazoline hybrid and synthesized its analogues inorder to discover a new class of antileishmanial agents.



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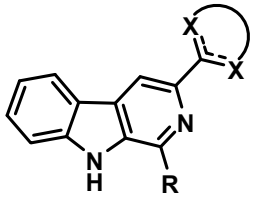

(II)

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PP 52

MICROWAVE ASSISTED SOLVENT-LESS SYNTHESIS OF 3-ALKYL-5-ARYL-TETRAZOLO-[1, 5-*a*] PYRIDINES

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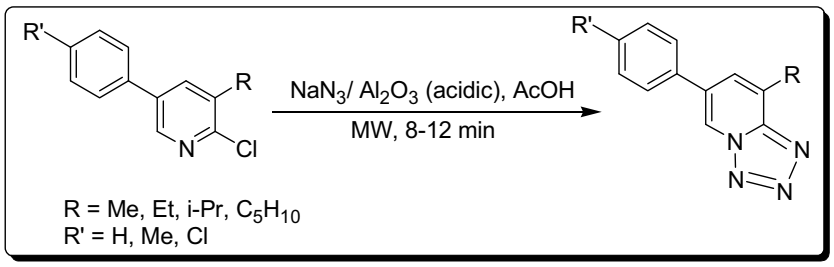
Most of the natural and synthetic biologically active compounds belong to nitrogen containing heterocycles and they constitute an important class of pharmacophores in medicinal chemistry [1], [2]. It has been found that tetrazole-fused nitrogenous heterocycles exhibit wide biological activities. Tetrazoloquinolines, for example, exhibit anti-inflammatory, antibacterial and antitumour properties [3] and tetrazolo [1, 5-*a*] pyridines act as anti bacterial agents and show potent and selective inhibition of the two well known herpes viruses HSV-1 and HSV-2. Literature revealed that tetrazolopyridines are conventionally prepared by prolong heating of 2-halopyridine with NaN_3 in a polar solvent [4]. In continuation of our interests for developing newer strategies for pyridine analogues, [5] herein, we report an efficient solvent-less methodology for the synthesis of tetrazolo [1, 5-*a*] pyridines from 3-alkyl-2-chloro-5-arylpyridines in high yield under microwave irradiation.



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PP 53

DESIGN AND SYNTHESIS OF POTENT ANTITUBERCULAR AGENTS BY USING GREEN APPROACH.

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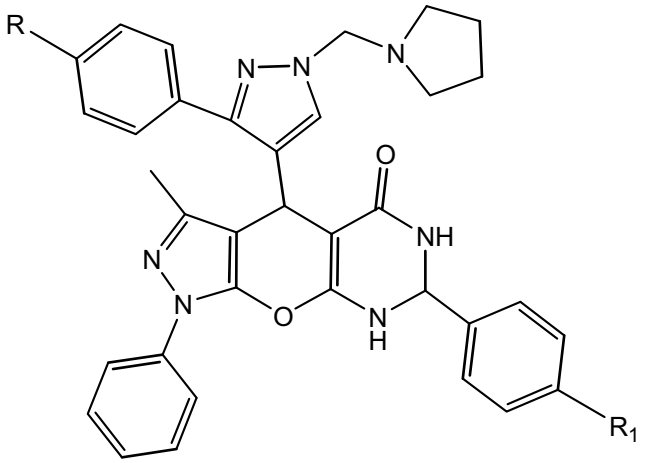
The extensive demand for cleaner and sustainable environment is forcing chemist to use less hazardous material. This regards, PEG-400, Bleach earth clay and Amberlyst are attracted considerable amount of interest due to their less toxic behavior.

In the present communication a green and efficient synthesis of some novel 6-amino-4(substituted)-3-methyl-1-phenyl-1,4-dihydro-pyrano(2,3-c)Pyrazole carbonitrile were described by the one-pot condensation of 3-methyl-1-phenyl-1H-pyrazol-5-ones with substituted heterylaldehydes, malononitrile in catalytic amount of bleaching earth clay (pH12.5) in Polyethylene glycol (PEG-400) as green reaction solvent to obtain bifunctionally active compound which were used as the key intermediate for the synthesis of some novel 4-(substituted)-7(substituted phenyl)3-methyl-1-phenyl-4,6,7,8-tetrahydro-1H,-9-oxa,1, 2, 6, 8-tetrazacyclopenta-5-one(b)-napthlene-5-one derivatives through its reaction with substituted benzaldehyde in the presence of IRA-Amberlyst-16WET as catalyst in Polyethylene glycol(PEG-400) gave corresponding products in high yield and purity. The chemical structures of newly synthesized compounds were confirmed by the spectral data. All the compounds of series were screened for their antitubercular activity studies; the result revealed that most of the compounds show potent antitubercular activity.



PP 54

NEW SUBSTITUTED THIOPHENE-SULPHONAMIDE THIOZOLYL PYRAZOLINE DERIVATIVES AS POTENT ANTITUBERCULAR AGENTS.

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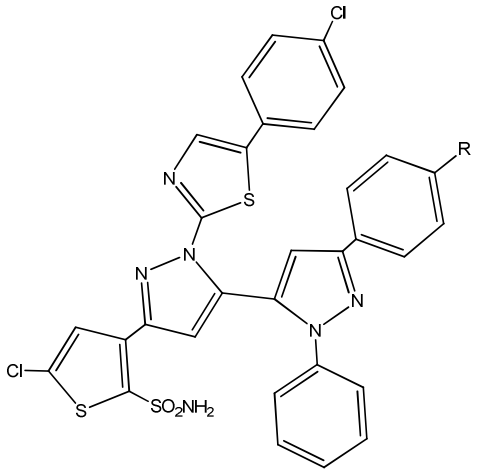
Increasing number of multidrug resistant tuberculosis (MDR-TB) extensively drug resistant (XDR-TB) and most recently emergence of totally resistant (TDR) tuberculosis (TB) is alarming and still one of the major causes of bacterial infection. Due to the unusual structure and chemical composition of the mycobacterial cell wall, effective TB treatment is difficult which makes many antibiotics ineffective and hinders the entry of drug. With approximately 33% of infection tuberculosis is still the second most imperative infectious disease world wide the most important reason for this is drug resistant TB(MDR,XDR) persistent infection (latent TB) and synergism of TB with HIV , further more no any new chemical entity has come in picture in last 40 years. New data available from the recently sequenced genome of the mycobacterium and application of method as of modern drug design promises to bring significant development in the against this disease.

Interest in the search of green chemistry routes using eco-friendly solvent such as Polyethylene glycol (PEG-400) for the synthesis of potentially active antimycobacterial agents.The pyazoline and thiazoline derivative are known for their broad spectrum such as antitubercular, antibacterial, anti-inflammatory and antidiabetic pharmacological activity. These observations have promoted us to design and synthesis of new kind of active molecule having thiophene-sulphonamide thaizolyl pyrazoline derivative by using greener methods and all compounds were tested for antituberculosis activity, most of the compounds were found to have significant activity.



PP 55

ROLE OF CHEMISTRY IN ARCHAEOLOGY: EMERGING TREND OF ARCHAEO-CHEMISTRY

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As discipline archaeology studies human past on the basis of verbal and nonverbal material remains which divided into Artefacts & Ecofacts- (Relics such as standing monuments, sites, structures, pottery, tools, ornaments, biological remains, etc). With the introduction of new archaeology in 1960, archaeologists looked towards the subject as multidisciplinary as well as interdisciplinary. Various scientific techniques are come into use to find out the answer of many questions which were unanswered before some decades. Chemistry as a helping branch for archaeology provided different dating techniques which helped to get older and older dates for the artefacts.

Present paper aims to focus on the various aspects of archaeo-chemistry and how these chemical sciences generated some new data with help of different scientific aids used in archaeology. This would also focus on the various shades of both the branches and combined efforts for the better knowledge for the future studies.

PP 56

SYNTHESIS, CHARACTERIZATION AND MICROBIAL ACTIVITY OF SCHIFF BASES AND THEIR CO^{II}, NI^{II}, CU^{II} AND ZN^{II} METAL CHELATES

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Three Schiff bases derived from 4-(P-bromo-phenyl)-2- aminothiazole and R-substituted 2-hydroxy- acetophenone (R = H, 5 – CH_3 and 5 – Cl) and transition metals. (Co^{II}, Ni^{II}, Cu^{II} and Zn^{II}). The complexes were characterized by elemental analysis, molar conductance, magnetic susceptibility spectral studies. (IR and UV). The metal coordinates with Schiff base nitrogen atom, azonitrogen atom and phenolic oxygen atom. The NNO donor ligand acts as tridentate ligand in all complexes. The complexes have 1:2 (metal ligand) stiochiometry and an octahedral geometry.

Proton ligand and metal ligand stability constants have been determined by PH metrically at room temperature at constant ionic strength (I = o.1m $NaClO_4$) in 50:50 (%) ethanol water medium using calvin Bjerrum PH metric technique. The order of stability constant of the complexes have been proposed which is in accordance with the order suggested by Irving Williams.

Thermodynamic parameter ΔH, ΔG and ΔS also calculated at elevated temperatures (25, 35 and 45^0 C) ΔH and ΔG are negative, while ΔS are positive.

The Schiff bases whose antibacterial and antifungal activities are checked and found that they are active and inactive respectively.

PP 57

SYNTHESIS OF 1-(4-NITRPOHENYL-2-(CHROMON-3-YL)ETHENES UNDER MW ASSISTANCE AND SOLVENT FREE CONDITIONS

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4-Oxo-4H-1-benzopyran-3-carboxaldehydes **1** were condensed with 4-nitrophenyl acetic acid **2** in the presence of anhydrous potassium carbonate under solvent free conditions and M.W. assistance to yield 1-(4-nitrpohenyl-2-(chromon-3-yl)ethenes **3**. The new heterocyclic compounds were characterized by spectral methods and scanned for antimicrobial activities.

PP 58

SYNTHESIS AND CHARACTERIZATION OF 1, 2, 3-TRIAZOLE CONTAINING PIPERAZINE DERIVATIVES *VIA* HUISGEN 1,3-DIPOLAR CYCLOADDITION REACTION FOR BIOLOGICAL EVALUATION

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Sharpless published a landmark review [1] describing a new strategy for organic chemistry, using "Click Chemistry". Among the listed click reactions, Huisgen 1,3-dipolar cycloadditions between an azide and an alkyne has been widely explored due to, among others, its efficiency, versatility and inertness towards other functional groups **(Figure 1).** Triazoles have been shown to possess a number of desirable features in the context of medicinal chemistry.

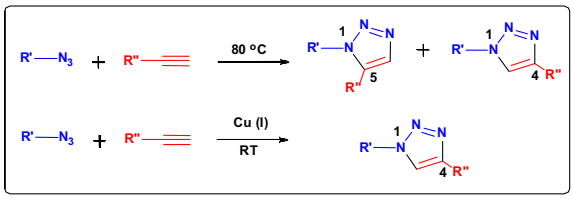

Figure 1: Schematic illustration of the azide-alkyne Huisgen 1,3-dipolar cycloaddition reaction

To explore a versatile methodology for a rapid and direct simple and efficient route to synthesis piperazine derivatives we have undertaken to systematically assess the contribution of triazole to the biological activity by a quantitative structure–activity relationship (QSAR) study [2].

Thus we have designed and synthesized a series of novel piperazine derivatives, characterized by spectra data like FT-IR and NMR. These compounds containing azide functional group has been reacted with alkyne in aqueous medium at room temperature and then studied for the in vitro biological evaluation.

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PP 59

SKELETAL DIVERSE SYNTHESIS OF *N*-FUSED POLYCYCLIC HETEROCYCLES VIA THE SEQUENCE OF UGI- TYPE MCR AND CuI CATALYZED COUPLING/TANDEM PICTET-SPENGLER REACTION

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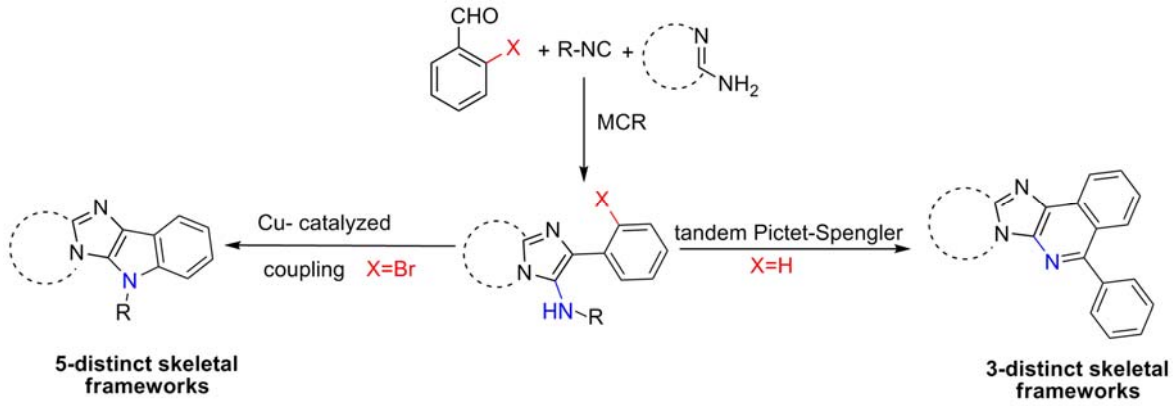
Nitrogen containing polycyclic molecules and analogues has attracted much attention due to their presence in biologically active natural products and pharmaceuticals [1]. Several diversity oriented syntheses of *N*-fused polycyclic heterocycles have been demonstrated but most are based on point diversity within the same library and usually involve time consuming sequential multi-step syntheses, suffer from low yields and/or poor precursor scopes [2]. We have developed a new strategy for the syntheses of skeletal diverse *N*-fused polycyclic compounds via an Ugi-type MCR [3][4][5] followed by CuI catalyzed coupling reaction or tandem Pictet–Spengler reaction[6][7]. This two step sequence provides eight distinct skeleton of fused {6-5-5-6}, {5-5-5-6}, {6-5-6-6} and {5-5-6-6} ring systems for the application in medicinal chemistry and chemical genetics.



PP 60

MICROBIAL GAS SENSING PROPERTIES E-COLI WITH MIXED METAL CATALYST $MgFe_2O_4$

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Semiconductive nanoparticles of Bactria as E.coli with catalyst $MgFe_2O_4$ were synthesized by a solution combustion technique. The process was a convenient, environment friendly, inexpensive and efficient method for synthesis of E.coli nanoparticles. The synthesized materials were characterized by TG/DTA, XRD, and TEM. Conductance responses of the nanocrystalline E.coli with catalyst $MgFe_2O_4$, thick film were measured by exposing the film to reducing gases like Acetone, Ethanol, Ammonia (NH_3), Carbon dioxide (CO_2), and Liquefied petroleum gas (LPG). It was found that the E.coli sensors exhibited various sensing responses to these gases at different operating temperature. Furthermore, the sensor exhibited a fast response and a good recovery. The results demonstrated that E.coli with catalyst MgFe2O4 can be used as a new type of gas-sensing material which has a high sensitivity and good selectivity to various gases at low ppm.

PP 61

SYNTHESIS OF D-*GULO*- AND L-*MANNO*-HOMONOJIRIMYCIN FROM D-GLUCOSE

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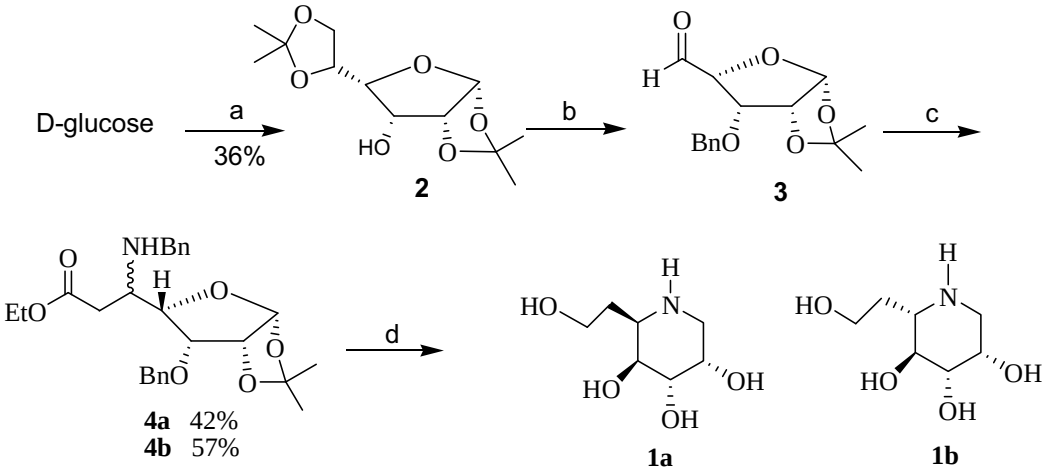
Nitrogen incorporated polyhydroxylated carbocyclic ring systems, commonly known as iminosugars, are of great importance as they exhibit significant glycosidase inhibitory activity. In the search for structure-activity relationship, a number of six and five member iminosugar analogues were synthesized and evaluated for their biological activity. These iminosugars selectively inhibit glycosidase that modify glycoconjugates by hydrolyzing glycosidic linkages and are therefore potential candidates as antiviral, antibacterial or, antimetastatic reagents. Thus, in the synthesis of homonojirimycin analogue **1a** and **1b** required □-L-*lyxo*-pentodialdose **3** was prepared from diacetone-D-glucose, which on Wittig olefination, conjugate addition of N-benzylamine afforded distereomeric **4a,b** (42:58). Individual reaction of **4a** and **4b** with LAH, H_2, Pd/C, ammonium formate, Cbz protection and deprotection of 1,2 acetonide in TFA-water followed by reductive amino cyclization under hydrogenation condition afforded D-*gulo*-homonojirimycin **1a** and L-*manno*-homonojirimycin **1b.**



Scheme .a) i) acetone,I_2,ii) pcc, iii) $NaBH_4$, iv) $(CH_3CO)_2O$, pyridine,DMAP, iv)LAH, THF, 0^oC. b) i) NaH, BnBr, 96%; ii) 20% TFA-H_2O, 82%; iii) $NaIO_4$, CH_3COCH_3, 89%; c) i) PPh_3=CHCOOEt, 99%; ii)$BnNH_2$,99%; iii)LAH, iv)H_2,Pd-C; v) Cbz, K_2CO_3; d) i) TFA-H_2O ii) H_2, Pd-C, 70%.

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PP 62

THIOCYANATION OF AROMATIC COMPOUNDS BY USING IONIC LIQUID

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An efficient, rapid thiocyanation of Aromatic compounds using ammonium thiocyanate has been developed by using ionic liquid under mild condition. The corresponding aryl thiocyanates are produced in excellent yields.

In recent years, ionic liquids have received great attention in chemistry as they have been catalytic species and alternative solvents to replace the traditional solvents. These versatile properties of ionic liquids prompt chemist to carry out numerous organic reaction in the ionic liquid [1].

Aryl thiocyanates are important synthetic precursors for the preparation of sulfur-containing organic compounds. The thiocyanato group occurs as an important functionality in certain anticancer natural products, [2] also these are intermediates for a preferred synthetic route to several types of thiazoles, [3] this functional group can be used as a masked mercapto group. Aryl thiocyanates have found a wide variety of applications as insecticides, [4] biocidal, [5] antiasthmatics, [6] vulcanization accelerators, [7] and starting materials for the preparation of heterocycles. Here we report a novel, rapid and eco-friendly method for the synthesis aryl thiocyanates, using ionic liquid.

Scheme:

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PP 63

IN VITRO ANTHELMINTIC ACTIVITY OF LEAVES OF LANTANA CAMARA L.

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Helminthes infections are among the most common infections in man; in developing countries they pose a large threat to public. Helminths parasite infections are global problems with serious social and economic repercussion in third world countries. The diseases affect the health status of large fraction of the human population as well as animals.

These infections can affect most population in endemic areas with social consequences. *Lantana camara* L. is regarded both as notorious weed and popular ornamental garden plant and has found various uses in folk medicine in many parts of the world. *Lantana camara* produces a number of metabolites in good yield and some have been shown to possess useful biological activities.

The study was undertaken to evaluate anthelmintic activity of different successive extracts namely ethanolic, ethyl acetate and aqueous using *Pheretima posthuma* as test worms. The different concentrations (0.1%, 0.3% and 0.5%) of various extracts were tested in the bioassay which involved determination of the time of paralysis (P) and time of death (D) of the worms. Albendazole was included as standard reference and normal saline as control.

The results of present study indicated that the crude ethanolic extract and aqueous extracts significantly demonstrated paralysis and also caused death of worms in dose dependent manner, as compared to standard reference albendazole. While ethyl acetate extract showed weak anthelmintic effect further studies are in process to isolate the active principles responsible for the activity.

PP 64

GREEN & ENVIRONMENTALLY BENIGN PROCESS FOR SYNTHESIS OF PYRAZOLE CHALCONES BY USING PEG – 300 AS A GREEN SOLVENT

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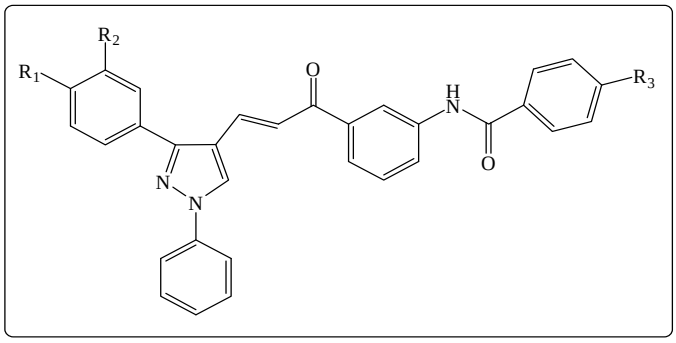
Pyrazole Chalcones constitute an important class of natural products which serve as precursors for the preparation of various flavonoids and exhibit interesting pharmacological activities[1]. A series of fluoro substituted chalcones have been synthesized by reacting N-(3-Acetyl-phenyl)-4-fluoro-benzamide with different substituted pyrazole aldehydes by using polyethylene glycol (PEG-300) as a green solvent[2,3]. PEG's are preferred over organic solvents due to inexpensive, easily degradable, low toxicity and recyclable. The advantages of this protocol are easy workup, excellent yield, mild reaction and avoidance of volatile organic solvent.



We wish to report a practical and efficient green method to prepare pyrazole Chalcones. Thus this green solvent (PEG-300) could be used for the synthesis of wide variety of pyrazole Chalcones under safe condition. The structure of the compounds were established by IR, ^{1}HNMR and LCMS spectral analysis

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PP 65

SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL EVALUATION OF FLUORO SUBSTITUTED PYRAZOLE CHALCONES AS ANTIOXIDANT - ANTIMICROBIAL AGENTS

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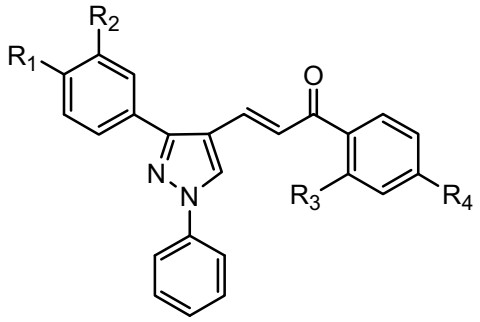
The chemistry of Chalcones has displayed intensive scientific interest due to their biological and industrial applications.Chalcone, an important intermediate of flavonoid synthetic pathway exerts a great deal of pharmacological activities viz. antimicrobial, anti-inflammatory, antioxidant[1], anticancer,antimalarial, anti-allergic etc. On the other hand, pyrazoles are of interest as potent bioactive molecules.

In continuation of our work on synthesis of some new bioactive heterocyclic compounds herein we report a series of synthesis of fluoro substituted pyrazole Chalcones by the condensation of fluoro substituted acetophenone with different substituted pyrazole aldehydes in polyethylene glycol(PEG-400)[2] as a green solvent.These synthesized compounds were characterized by spectral analysis(IR,1HNMR,LCMS). All the compounds were screened for antioxidant (DPPH, SOR, and OH radical scavenging assay) and antimicrobial activities against some pathogenic bacteria and fungi.



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PP 66

DEVELOPMENT AND VALIDATION OF A STABILITY INDICATING UPLC ASSAY METHOD FOR DETERMINATION OF CHLORHEXIDINEGLUCONATE AND LIDOCAINE HYDROCHLORIDE IN THROAT SPRAY

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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 chlorhexidinegluconate 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 Chlorhexidinegluconate 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 Chlorhexidinegluconate. 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 Chlorhexidinegluconate 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 chlorhexidinegluconate and lidocaine hydrochloride and the assay can thus be considered stability indicating.

PP 67

HIGHLY RAPID AND DIRECT SYNTHESIS OF DIARYL SULFOXIDES

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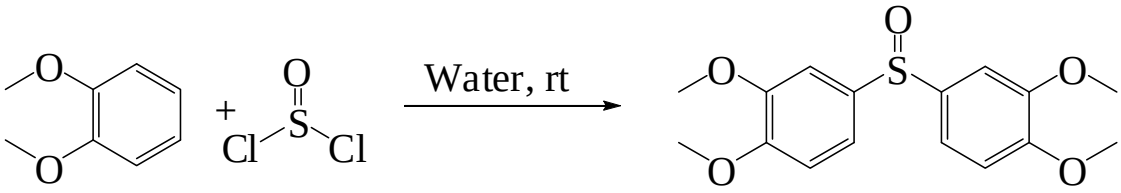
In organic synthesis increasing attention is being focused on reaction in aqueous media [1]. When solvent must be used, water is the most acceptable in term of cost and environmental impact. Most catalyst and reagent are deactivated or decomposed in water and in general organic compounds are insoluble in water. therefore, carrying out organic reactions in water poses important challenges in area of reaction design. Sulphoxides and sulfones are interesting functional groups possessing manifold reactivity for conversion of a variety of organic sulphur compounds in the field of drug and pharmaceuticals [2].

We wish to highlight our results on the electrophilic sulfinylation of arenas with thionyl chloride and 10/ of water. Thus treatment of several arenas reacted with thionyl chloride to give the corresponding diaryl sulfoxides in good to excellent yield, mild reaction condition, greater selectivity, short reaction time and operational simplicity.



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PP 68

DEVELOPMENT OF VARIOUS THIOSEMICARBAZONE REAGENTS FOR EXTRACTIVE SPECTROPHOTOMETRIC DETERMINATION OF Pd (II)

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Solvent extraction method is the method of analysis of ions, impurity detection, enrichment, and complex formation. Thiosemicarbazone reagents form colored complexes with metal ions. These complexes are also found to have biological activities, which have medicinal values in the treatment of diseases like Influenza, Protozoa, Small pox and some tumors and which also have antitubercular activity. Metal chelates of these reagents are used as pesticides and fungicides in Agriculture. These reagents forms stable complexes with Pd(II).It is found in pharmaceutical, commercial, agricultural and analytical samples. Among the various analytical methods of determination of Pd(II).,at micro level, the spectrophotometric methods are less expensive and more sensitive. Literature survey reveals that only few thiosemicarbazone reagents are synthesized for extractive spectrophotometric determination of Pd(II). The present work constitute the development of various thiosemicarbazone reagents for such determination of Pd(II) and selection of a special reagent which will extract Pd(II) at working range of P^H and with minimum folds of moles of reagent, with more stability and to develop a practical method for determination of Pd(II).To develop the practical method by use of selected thiosemicarbazone which is applied for pharmaceutical, commercial, and analytical samples of toxic Pd(II). All developed thiosemicarbazones extract Pd(II) with good stability of complexes. The heterocyclic ligands shows greater stability of Pd(II) complexes. The selected heterocyclic ligand (E), Indole-3-aldehyde thiosemicarbazone (I3ATS) extract Pd(II) at 5.5 - 6.5 range of P^H and with about 3 folds of moles of reagent for complete color development.

PP 69

CONDUCTING POLYANILINE NANOFIBER NETWORKS PREPARED BY DOPING INDUCTION OF DODECYL BENZENE SULFONIC ACID (DBSA)

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Recent progress in the processing of conducting polyaniline (PANi) protonated with functionalized sulfonic acid (such as DBSA) has enabled the fabrication of high quality, homogeneous films with excellent surface quantity.

Branched nanofibers of conducting polyaniline (PANi) buried in the crystal of dodecyl benzene sulfonic acid (DBSA) were prepared from an m-cresol solution of PANi and excessive DBSA. The X-ray diffraction patters of DBSA doped PANi showed high crystallinity. Proper formation of the polyaniline and incorporation of DBSA into the polymer chain film in a conducting form was confirmed from the FTIR studies. The peaks at 1,591 and 1,497 cm^{-1} originate from aromatic C-C stretching vibrations whereas those at 1,307 and 1,167 cm^{-1} are due to aromatic amine stretching. The peak at 832 cm^{-1} comes from the out of plane hydrogen deformation of aromatic rings in PANi unit sequences.

The electrical conductivity of these films has been measured as a function of temperature between 300-500K. Pure PANi exhibits room temperature conductivity of 5.32 $x10^{-7}$ S/cm and PANi – DBSA (50%) exhibit 2.92 $x10^{-6}$ S/cm. UV- visible absorption spectra of PANi(EB) thin film gives absorption band at ~ 461 nm assigned as the benzene π-π^* transition. A steadily increasing free carrier tail starting from ~756 nm to the near –IR region is observed for DBSA doped PANi film with a shoulder at ~900 nm.

PP 70

FACILE AND EFFICIENT ROUTE FOR PREPARATION OF POLYPYRROLE-ZnO NANOCOMPOSITES: MICROSTRUCTURAL, OPTICAL AND CHARGE TRANSPORT PROPERTIES

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Polypyrrole (PPy) nanocomposites reinforced with zinc oxide (ZnONPs) nanoparticles were fabricated by spin coating method. The polymer nanocomposite films were characterized by X-ray Diffraction (XRD), Scanning electron microscopy (SEM), Fourier transform infrared (FTIR), UV-vis spectroscopy and Four probe technique. The results were compared with polypyrrole film. Powder X-ray diffraction analysis demonstrates the crystalline structure of ZnO nanostructures, as well as their corresponding nanocomposites. The SEM images of the nanocomposites show uniform distribution of the ZnO NPs in the PPy matrix. The overall grain size was found to change in nanocomposite films. In the FTIR spectra, the characteristic peaks of pure PPy are observed to shift to higher wave number revels the different interfacial interactions between the ZnO NPs and the PPy matrix. In the UV-vis spectra, absorption peak of PPy shifts to lower wavelengths indicating poor conjugation. The electrical resistivity of PPy-ZnO nanocomposites is observed to depend strongly on the particle loadings and the morphology.

PP 71

LITHOCHOLIC ACID BASED POLYESTERS: SYNTHESIS, CHARACTERIZATION AND RELEASE OF PARACETAMOL AS A MODEL DRUG.

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Polyesters containing lithocholic acid were synthesized by reaction of lithocholic acid sebacate [Bis(5β-cholan-24-oic acid 3α-yl)] with various diols such as PEG-400, PEG-600, PEG-800, 1,4-butane diol and 1,6- hexane diol using dibutyl tin oxide (DBTO) as a catalyst. These polymers were characterized by IR and ^{1}H NMR and their solubility was checked in various solvents. These polymers were used as a matrix to study the release of paracetamol as a model drug at two different pH (1.2 and 7.4). The release studies showed that at pH 1.2 the release of the drug was slow i.e. 37%, 32%, 31%, 26% and 28% after 30 hours but at pH 7.4 the release of the drug increases i.e. 89%, 80%, 81%, 77% and 60% after 30 hours. Thus, the results indicate that the polymers could be good candidates as matrix for sustained release of drugs

PP 72

SYNTHESIS AND FLUORESCENT STUDY OF 2,3-DISUBSTITUTED MALEIC ANHYDRIDE DERIVATIVES FOR BIOLOGICAL APPLICATIONS

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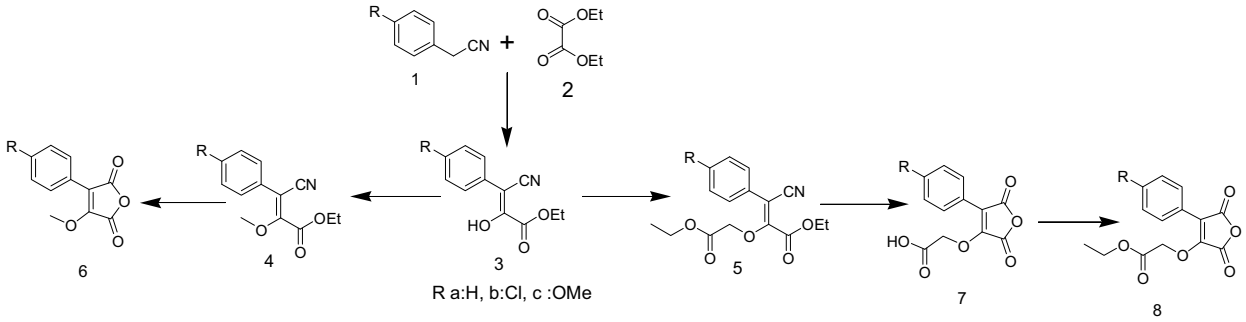
Since last two decades ,synthesis of fluorescent material has attracted the researchers from the area of biochemistry, clinical chemistry, and analytical chemistry. In the area of biochemistry ,the fluorescence has found the numerous applications to investigate the structure and dynamics of the living systems[1,].Now a days in the clinical diagnosis fluorescence has replaced the harmful radioactive tracers .The use of fluorescence eliminates the radioactive material and their cost of proper disposal. Human Genome Project were made practical by use of fluorescent labels [2,] In analytical methodologies , use of fluorescence is increasing day by day because sensitivity of fluorescence is far greater than common UV technique. viz. Amino acids are poor UV absorbing compounds hence their fluorescent derivatisation is employed [3]

Therefore we thought to synthesise [4] the new material for use in fluorescence application with desired side chain and photophysical properties. 2-Aryl-3-alkoxy maleic anhydride derivatives were synthesized in good yields (Scheme-I). The compounds 6, 7 and 8 shows fluorescence in visible region with high quantum yield.(Table 1).



Scheme- I

Table 1 **:** UV and Fluorescence data.

Compound	6a	6b	6c	7a	7b	7c
UV λmax(nm)	341	365	374	340	346	374
λ em (nm)	433	349	478	428	435	482
ϕ_f	0.78	0.75	0.81	0.87	0.90	0.78

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PP 73

SYNTHESIS OF SOME NOVEL 3-CYANO-5-METHYL PYRAZOLO (1,5-A)PYRIMIDINE DERIVATIVES

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A series of 2,7-disubstituted 3-cyano-5-methyl pyrazolo(1,5-a)pyrimidine derivatives were synthesised by reacting 5-substituted 3-amino pyrazole 4-carbonitriles with 1-substituted 3-dimethyl amino but-2-en-1-ones. 5-substituted 3-amino pyrazole 4-carbonitriles were prepared from substituted piperdine, bis (methyl thio) methylene malanonitrile and hydrazine hydrate. 1-substituted 3-dimethyl amino but-2-en-1-ones were prepared from 2-acetyl derivatives and dimethyl acetamide dimethyl acetal. Structures of these compounds were established by IR, NMR, Mass spectra. Further study is under progress to understand their anxiolytic activity in our laboratory.

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PP 74

ACCIDENTAL DISCOVERY OF A 'LONGER-RANGE' VINYLOGOUS PUMMERER-TYPE LACTONIZATION: FORMATION OF SULINDAC SULFIDE LACTONE FROM SULINDAC

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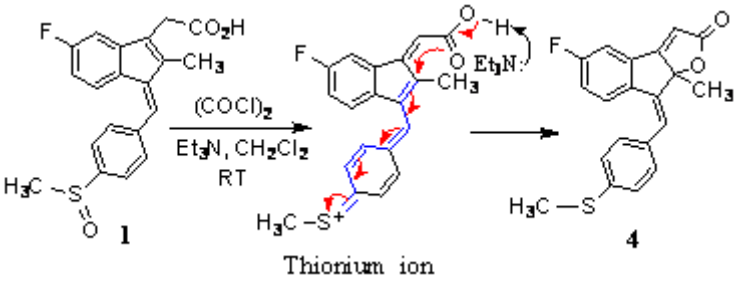
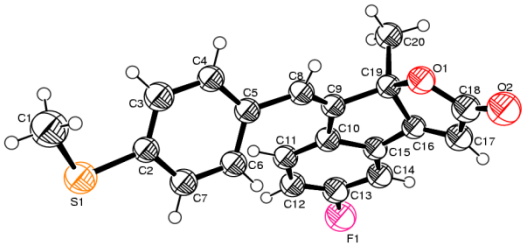
Unexpected formation of sulindac sulfide lactone (**4**) occurred when sulindac (**1**) was treated with oxalyl chloride and triethylamine at room temperature. Structurally analogous sulindac sulfide and indomethacin did not undergo such lactonization under similar reaction conditions. We believe that the sulfoxide function in sulindac plays a pivotal role possibly via a 'longer-range' vinylogous Pummerer-type reaction[1] as a driving force for the observed lactonization. We have discovered the interesting 'longer-range' vinylogous Pummerer-type lactonization process wherein we obtained the sulindac sulfide lactone (**4**) as the major product. Although a few examples of extended or 'long-range' (i.e., involving a conjugated chain of 3 to 5 atoms) vinylogous Pummerer-type cyclizations are reported in the literature,[2] as far as we know, ours is the first example of a vinylogous Pummerer-type lactonization wherein such a 'longer-range' (i.e., consisting of a conjugated chain of 7 or 9 carbon atoms) process is involved. We have also confirmed the structure of lactone **4** by a single crystal X-ray analysis.[3]





X-ray structure of **4**

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PP 75

SYNTHESIS AND CYTOTOXIC EVALUATION OF SOME 3-SUBSTITUTED-2-OXINDOLE DERIVATIVES AGAINST MURINE AND HUMAN TUMOUR CELL LINES

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Cancer is a disease characterized by uncontrolled proliferation and spread of abnormal forms of the body's own cell(Zhang)[3]. As part of our ongoing studies concerning the preparation of potential anti tumour compounds, we were interested in the synthesis of indoline-2- one derivatives(*Sassatelli et al.,)*[1], (*Messaoudi et al.,*)[2]. A series of 3-substituted-2-oxindole derivatives have been synthesized by reacting isatin with benzoyl hydrazide in good yield. The structure of these compounds were established by IR, H^1 NMR,MASS spectras. The selected compounds were evaluated for their preliminary cytotoxic activity against the murine leukaemia cells,human T-lymphocyte cells and human cervix carcinoma cells. The results showed that **SKS 200** more potent cytotoxic (0.66 to 1.0µm) on composition to standard (2.1 to 3.2µm) its further study under progress to understand its cell cycle study, MoA etc in our laboratory.

PP 76

INVESTIGATION OF MINERAL COMPOSITION PRESENT IN BARLERIA PRIONITIS

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Barleriaprionitis plant finds a lot of reference in the ayurvedic literature, but its correct identity is not know today. There are several plants listed under the name of Barleria among them *Barleriaprionitis* selected for study as they have not been much investigated. Their morphological characters are capable of vegetative reproduction when cuttings or stem fragments encounter a suitably moist environment that allows them to start growing roots. Barleria can probably also reproduce vegetative. The amount of tannin was confirmed by qualitative and quantitative methods. Further mineral analysis was carried out according to standard procedure using various methods. In conclusion, it can be suggested that plant have significant amount of minerals in leaves, stem and roots for development as useful remedies.

PP 77

SYNTHESIS AND ANTIMICROBIAL ACTIVITY OF SOME IMIDAZO [2,1-B]-1,3,4 THIADIAZOLE DERIVATIVES

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A series of 2,5,6- trisubstituted imidazo[2,1-b]-1,3,4-thiadiazole derivatives have been synthesized by reacting with 2-amino-5-benzyl-1,3,4- thiadiazoles and an appropriate 4-substituted/unsubstituted phenacyl bromide (Karki et al.)[1]. Further 5-formyl/5-bromo/5-thiocyanate derivatives were synthesized inorder to study the effect of these substituents on biological activity.Structures of the compounds were established by IR, ^{1}H NMR, Mass spectras. The selected compounds were evaluated for their preliminary invitro antimicrobial activity against few strains of some organisms like *E.coli, staphylococcus aureus, E.faecalis, klebsiella*[2][3]. The results showed thatSKS-05[2-(4-chlorobenzyl)-6-(4-bromophenyl) imidazo(2,1-b)(1,3,4)thiadiazole],SKS-09[2-(4-chlorobenzyl)-6-(2,4-dichlorophenyl)imidazo(2,1-b)(1,3,4) thiadiazole compounds exhibited minimum inhibitory concentrations of 0.8,0.4 for *E.coli* and for SKS-22[2-(4-chlorobenzyl)-5-bromo-6-(4-bromophenyl)imidazo(2,1-b)(1,3,4)thiadiazole, MIC was found to be 0.2 for *E.faecalis*.

PP 78

PHYTOCHEMICAL INVESTIGATION OF GARLIC

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Garlic (*Allium sativum*), a member of the *Lily family*,used for specific food as a vegetable and for therapeutic purpose in folk medicines for thousands of years. Medicinal importance are antiviral effect,antibacterial, antimicrobial,anticancer effect,cholesterol lowering activity.Fresh garlic is a source of numerous vitamins, minerals and trace elements; garlic contains the highest sulphur than any other member of the allium genus. It contains about 0.5% of a volatile oil which composed of sulphur containing compound like diallyldisulphide, diallytrisulphide, methallallyltrisulphide. The isolation and characterization of the chemical compounds of*Allium sativum*were carried out. Isolation of organosulphar compound and free amino acid were carried out by column chromatography and thin layer chromatography. Ascorbic acid, protein and mineral composition were determined by estimation method. The isolated materials were identified by spectral data and were subjected chemotaxonomic importance and antimicrobial activity.

PP 79

SYNTHESIS AND BIOLOGICAL EVALUATION OF MANNICH AND SCHIFF BASES OF OXINDOLE DERIVATIVES

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2,3-dioxindole can be used to prepare a large variety of heterocyclic compounds, such as indoles and quinolines, and as a raw material for drug synthesis (Silva et al., 2001) [1]. Schiff bases and Mannich bases of isatin are known to possess a wide range of pharmacological properties including antibacterial, anticonvulsant, anti-HIV, antiviral and anticancer activity (karki et al., 2009) [2]. In view of these a series of Mannich bases of compounds were synthesized by reacting isatin with paraformaldehyde and diethyl amine. Further these Mannich bases were reacted with thiosemicarbazide/phenylthiosemicarbazide in good yield to get Schiff bases. Structures of these compounds were established by IR, NMR, and Mass Spectra. The selected compounds were evaluated for their cytotoxic (Baraldi et al., 2004) [3], antibacterial, antifungal activity. **5c** showed more potent cytotoxic (1.9-2.4 µM) activity and **5h** showed moderate (4.6-9.5 µM) cytotoxic activity against Murine leukemia cell line (L1210), human molt4/C8 and CEM T-lymphocytes in comparison to standard Melphalan (2.1-3.2 µM) and compounds **5d** and **5f** showed moderate antibacterial activity (zone of inhibition 21-30mm) against *S.aureus, B.subtilis, E.coli* in comparison with Ofloxacin (zone of inhibition 31-36 mm). Compounds **5a** and **5f** showed moderate antifungal activity (zone of inhibition 21-30 mm) against *S.typhi, A.niger, C.albicans* in comparison with standard Fluconazole (zone of inhibition 31-36 mm).

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PP 80

SYNTHESIS, BIOLOGICAL EVALUATION AND QSAR STUDIES OF SOME SUBSTITUTED BENZIMIDAZOLE DERIVATIVES.

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The pyridine substituted benzimidazoles synthesized from *p*-substituted acetanilides were evaluated and characterized by IR, H^1 NMR, MASS spectras (Puratchikody A *et al*.)[1]. The compounds SDS-59 and SDS-62 have shown significant activity at higher concentration {80-100 µm} against gram+ve bacteria(Ansari *et al*.)[2]. The computational 3D-QSAR studies of various benzimidazoles and its derivatives were designed to develop a statistically significant model by using Topomer CoMFA in the form of contour plots, showed the requirement of steric and electrostatic fields in the different regions of the fragments for better active molecules(*Cramer)[3]*. The r^2,q^2values obtained for three models evaluated are *e.coli*(0.725,0.627), *P.auregonisa* (0.843,0.610), *S.aureus*(0.827,0.636). All the models generated demonstrated the predictivity of activity which suggests that our approach may be beneficial for the discovery of novel molecules on the path of rational drug discovery.

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PP 81

PHYTO-TECHNOLOGICAL METHOD FOR TREATMENT OF SEWAGE THROUGH CONSTRUCTED WETLAND

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Water hyacinth (*Eichhornia crassipes*) is a free floating aquatic weed, which creates a serious problem of Eutrophication. Eutrophication is harmful to aquatic life and creates nuisance in irrigation, power generation and in domestic water usages. On the other, this weed is a valuable biotic resource with several properties in waste water treatment through its plant - root system called as Phyto-technology.

In the present investigation, water hyacinth is used for the treatment of sewage, because of its highest pollutant absorption capacity. It has been used for the treatment of sewage of Solapur city for recycling and reuse. The samples of sewage with different dilutions viz. 20%, 40%, 50%, 60%, 80% and 100% were tested for the treatment. The results reveal that the average reduction in Colour and odour is 100% and other parameters like COD and BOD_5 have been reduced up to 45.12% and 39.98 % respectively. Chlorides, Nitrates, TS, TDS and TSS are reduced by 7%, 60.15 %, 30.29%, 48.36 % and 38.76 % respectively along with the reduction in heavy metals like Cu, Ni, Co and Fe with maximum reduction in Co.

PP 82

IMPACT OF BILT GRAPHIC PAPER INDUSTRIAL EFFLUENTS ON SOIL TAL - INDAPUR, DIST - PUNE. (MAHARASHTRA)

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Bilt graphic paper industrial effluents disposal causing water pollution and Soil pollution. It is detrimental to human health and aquatic life, therefore it is needed to treatment plant such a effluent promote yield of agro productivity. Treated effluent providing nutrients, marginal fertility to soil. The pH of treated effluent is 7.8 therefore it is alkaline nature and high content of Ca, Mg, Chorine, Nitrate and TDS are observed. The impact of bilt graphic paper industrial effluent on soil is studied as analysis of effluents and analysis of soil prove that calcium and magnesium content is beyond the permissible limit and deficiency of iron and manganese content. Therefore ferrous sulfate and manganese sulfate is used for agro productivity of the soil.

PP 83

HIGHLY REGIOSELECTIVE AND STEREOSELECTIVE IODOCYCLIZATION REACTION OF ALKENE THIOUREAS: A NOVEL AND EFFICIENT APPROACH TO 3-THIA-1-DETHIACEPHAMS

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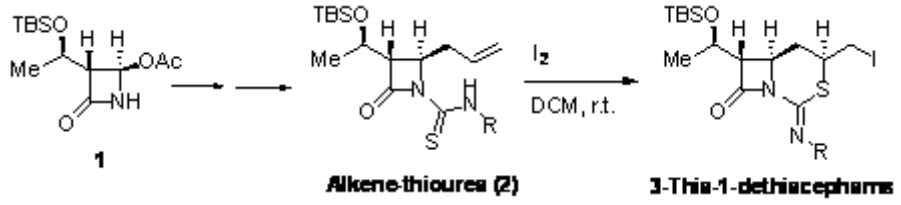
β-Lactam antibiotics, one of the most important contributions of science to human health, account for 50% of the world's total antibiotic market.[1] The continued effectiveness of these agents is threatened by increasing bacterial resistance and efforts have been made to meet this challenge by exploring new β-lactams by skeletal modification of naturally occurring β-lactam antibiotics. In this regard, it is surprising to note that, few reports are available for the synthesis of 3-thia-1-dethiacephams and thiazepines. The prepared compounds possessed functionality that compromised their biological activity. In continuation to efforts for the synthesis of bicyclic β-lactams,[1] we were interested in finding a new synthetic strategy for the preparation of novel bicyclic β-lactams.

Iodocyclization of an unsaturated C-C bond with a wide variety of nucleophiles, including N, O, and S nucleophiles, has been extensively studied and has become a powerful tool for the construction of various heterocycles.[2] In contrast, few reports on the iodocyclization reaction of alkene-thioureas are available in literature. Whereas, iodocyclization approach of alkene-thiourea was never described for the synthesis of bicyclic β-lactams. Herein, we report, the highly regioselective and stereoselective iodocyclization reactions of alkene-thioureas as an efficient protocol for the synthesis of bicyclic β-lactams. The reaction of alkene-thiourea **2,** synthesized from chiral acetoxyazetidinone **1**, with molecular iodine resulted in the formation of 3-thia-1-dethiacephams in good yields. The reaction afforded only six-membered bicyclic β-lactams, whereas seven-membered thiazepines were never observed under these reaction conditions.



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SYNTHESIS OF 3-THIA-1-DETHIACEPHAMS *VIA* REGIOSELECTIVE IODOCYCLIZATION OF ALKYNE-THIOUREAS

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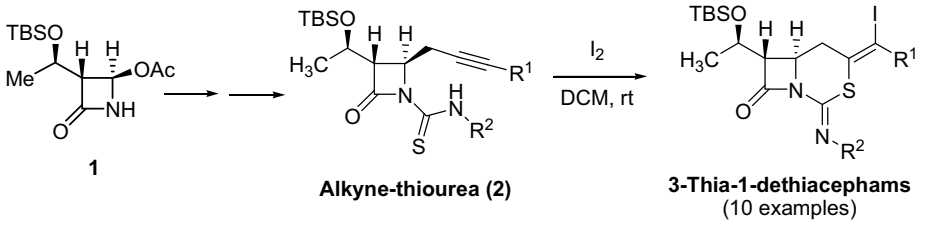
The β-lactam (2-azetidinone) skeleton is the key structural element of the most widely employed class of antibacterial agents, the β-lactam antibiotics.[1] Over the years, countless numbers of penicillin derivatives have been prepared and a variety of new β-lactam ring systems have been introduced due to the emergence of penicillin-resistant strains of bacteria. In this regard, it is surprising to note that, only a few reports are available for the synthesis of 3-thia-1-dethiacephams.

Iodocyclization of an unsaturated C-C bond with a wide variety of nucleophiles, including N, O, and S nucleophiles has become a powerful tool for the construction of various heterocycles.[2] In contrast, to the best of our knowledge, the iodocyclization reaction of alkyne-thioureas or allene-thioureas has never been described thus far. In continuation to our efforts for the synthesis of bicyclic β-lactams[1] herein, we report, the first highly regioselective and stereoselective iodocyclization reaction of β-alkyne-thioureas **2,** synthesized from chiral acetoxyazetidinone **1**, with molecular iodine to access 3-thia-1-dethiacephams. The reaction afforded six-membered bicyclic β-lactams, i.e.3-thia-1-dethiacephams as the only products whereas, the seven-membered thiazepines were never observed under these reaction conditions. The structure of the formed 3-thia-1-dethiacephams was elucidated by studies of IR, ^{1}H-, ^{13}C-NMR, COSY, HMQC, HMBC, NOESY and HRMS.



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PP 85

TITANIUM SILICATE-1 CATALYSED SIMPLE, EFFICIENT AND GREEN APPROACH FOR THE SYNTHESIS OF QUINOXALINES

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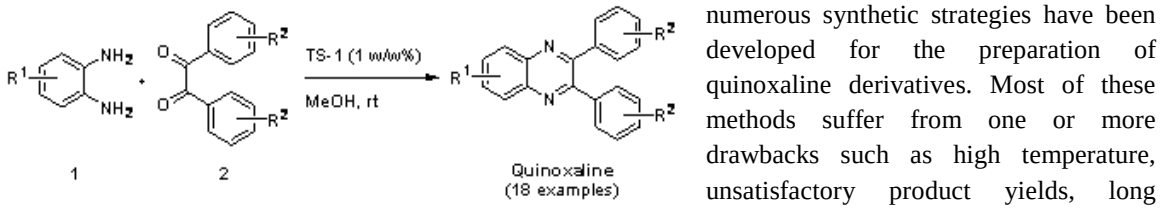
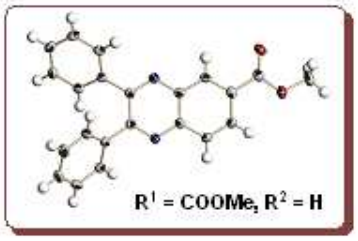
The quinoxaline and its derivatives constitute a very important, privileged class of nitrogen-containing heterocyclic compounds that shows various biological activities such as antiviral, anti-inflammatory, antiprotozoal, antihelmintic, herbicides, anticancer, antimalarial, and antidepressant activities.[1,2] Quinoxaline derivatives are present in different antibiotics such as echinomycin, levomycin, and actinoleutin, which inhibit the growth of Gram-positive bacteria. Beside its biological activities, it is used in the synthesis of organic semiconductors, dyes, and electroluminescent materials. Over the years, numerous synthetic strategies have been developed for the preparation of quinoxaline derivatives. Most of these methods suffer from one or more drawbacks such as high temperature, unsatisfactory product yields, long reaction time, use of hazardous solvent, critical product isolation procedure, and use of expensive catalysts, so a generalized method still remains an ongoing challenge. In recent days, zeolite catalyzed syntheses have attracted the attention of chemists because they are environmentally benign processes. As part of our research to develop more efficient and environmentally benign methods for organic syntheses using ecofriendly materials as catalysts, we have looked into the synthesis of Quinoxalines using catalytic amounts of TS-1 in methanol. Herein, we report, the reaction of o-phenylenediamines, **1** with substituted benzils, **2** using 1 w/w% of TS-1 catalyst in methanol readily afforded the quinoxalines. Simple reaction conditions, simple workup procedures and easy availability of the reagents make this route more attractive and economically viable. Further, the structure of the formed quinoxalines was confirmed spectroscopic methods and finally by X-ray crystallography.





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SYNTHESIS NOVEL TRIAZOLYL-XYLOSIDE DIMERS BY RUTHENIUM- AND COPPER-CATALYZED CLICK CHEMISTRY

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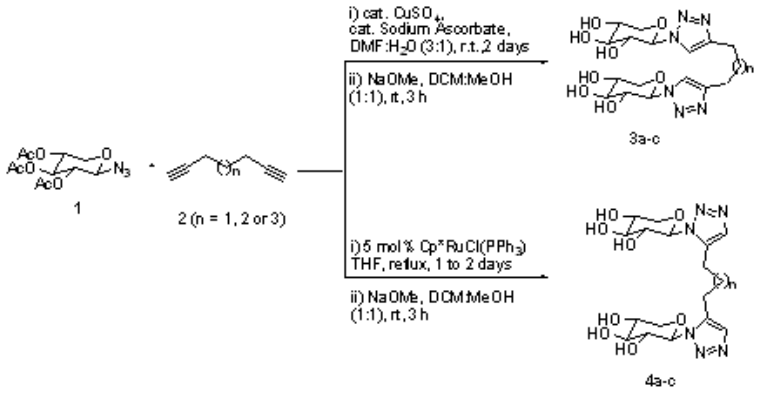
Proteoglycans (PGs) are composed of a core protein and one or more glycosaminoglycan (GAG) side chains such as chondroitin sulfate (CS) and heparan sulfate (HS).[1,2] In humans, these GAG side chains have been shown to regulate many biological functions, including wound healing, cell signaling, cell differentiation, angiogenesis, blood clotting, and tumor-cell migration. A common linkage tetrasaccharide, GlcAβ(1–3)Galβ(1–3)Galβ(1–4)Xylβ(1-O-Ser), is found between serine residues in core proteins and the GAG polysaccharide side chains. The first step in PG biosynthesis is xylosylation of certain serine residue of core protein. A specific linker tetrasaccaride is then assembled and serves as an acceptor for elongation of GAG chain. If the production of endogenous GAG chain is selectively inhibited, one could determine the role of these endogenous molecules in physiological and developmental functions in spatiotemporal manner. Biosynthesis of PGs is often blocked with the aid of nonspecific agents such as chlorate, a bleaching agent and brefendin A, a fungal metabolite, to elucidate the biological role of GAG chain.



Xylosides are known to prime GAG chain. Recently, Kuberan et al. have shown that a variety of triazolyl Xylosides, prepared by Cu-mediated click-chemistry, can selectively prime[1] or perturb[2] the GAG-chains biosynthesis. In this regard, for the structure-activity relationship study we have synthesized various triazolyl xyloside dimers **3** and **4** using Ru- and Cu-mediated click-chemistry, respectively. The synthesized compounds are expected to show interesting biological activities.

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ANTIPLASMODIAL ACTIVITY OF NOVEL KETO-ENAMINE CHALCONE-CHLOROQUINE BASED HYBRID PHARMACOPHORES

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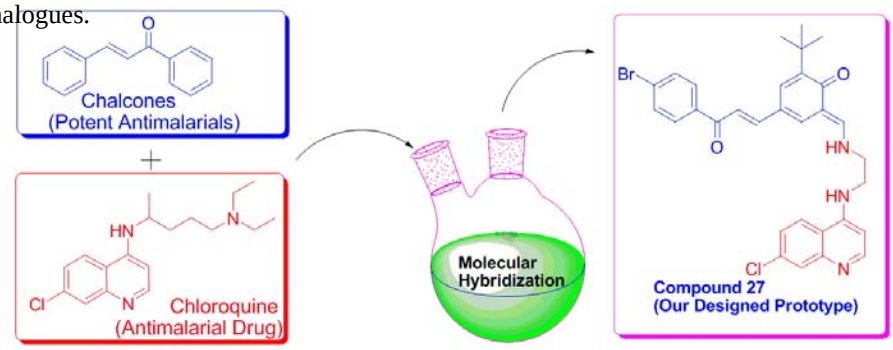
The problem of widespread malaria continues unabated worldwide, as the disease is present in over 100 countries and threatens half of the world's population. The resistance of *Plasmodium falciparum* to chloroquine and other antimalarial drugs and the adverse effects of some of the available antimalarial drugs have created an urgent need for new drugs that are safe and effective for the prophylaxis and treatment of malaria.[1,2] Adopting the medicinal chemistry hybridisation approach, we herein wish to report design, synthesis and antimalarial evaluation of chloroquine-chalcone hybrid pharmacophores. A series of novel keto-enamine chalcone-chloroquine based hybrids were synthesized following new methodology developed in our laboratory. The synthesized compounds were screened against chloroquine sensitive strain (3D7) of *P. falciparum* in an *in vitro* model. Some of the compounds were showing comparable antimalarial activity at par with chloroquine. Compounds with significant *in vitro* antimalarial activity were then evaluated for their *in vivo* efficacy in Swiss mice against *P. yoelii* (Chloroquine resistant N-67 strain), wherein compounds **25** and **27** each showed an in vivo suppression of 99.9% parasitaemia on day 4. Biochemical studies reveal that inhibition of hemozoin formation is the primary mechanism of action of these analogues.



Synthesis and antimalarial evaluation of novel chalcone-chloroquine hybrids is reported.

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ANTIOXIDANT ACTIVITY, ANTIFUNGAL ACTIVITY AND ACARICIDAL ACTIVITY OF *CRASSOCEPHALUM CREPIDIOIDES* (BENTH.) S. MOORE.

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The methanolic leaf extract of *Crassocephalum crepidioides* (Benth.) S. Moore obtained from Soxhlet extraction was examined for antioxidant, antifungal and miticidal activities. The antioxidant activity was determined by means of the DPPH radical scavenging test. The free radical scavenging activity was established as 71.26%. The extract was investigated for antifungal activity by agar-well diffusion method against plant pathogenic fungi *Colletotrichum gloesporioides* (Penzo) Sacc. of *Jatropha curcas* L. The extract of *C. crepidioides* showed 90% inhibition at 0.5% concentration level. The extract was investigated for miticidal activity against a serious pest *Oligonychus coffeae* Nietner of *Camellia sinensis* (L.) O. Kuntz. The extract showed 91% Mortality at 1% concentration. No mortality was observed in control. The present investigation revealed that methanolic extract of *C. crepidioides* has good antifungal and miticidal activities. However, further studies on bioactive compound are necessary for optimization of biological compounds.

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ANTITUBERCULOSIS AGENT DIAPORTHEONE B: TOTAL SYNTHESIS, ABSOLUTE CONFIGURATION ASSIGNMENT AND READY ACCESS TO ITS ANALOGS

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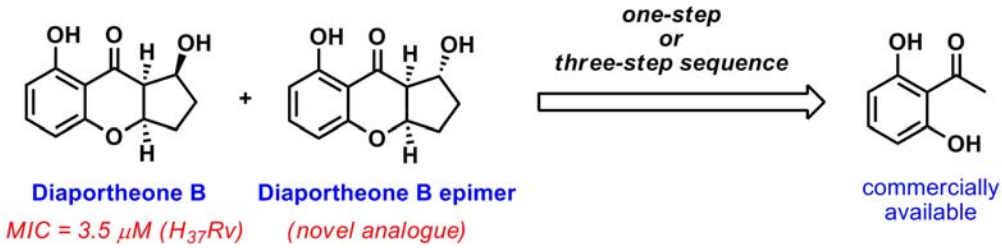
First and short synthesis of diaportheone B, an antituberculosis agent isolated from endophytic fungus *Diaporthe sp. P133* will be disclosed. We have achieved the synthesis in two complementary routes, one step and three-step sequence starting from bench-top chemicals. The absolute configuration of diaportheone B is determined by using the X-ray crystal structure analysis. In addition, we have prepared several close analogs of diaportheone B to determine their anti –TB potential which can provide a way forward for the medicinal chemistry program based on this novel chemotype.



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PP 90

A HIGHLY EFFICIENT AND GREEN METHOD FOR THE SYNTHESIS OF PYRIMIDO[4,5-*B*]INDOLE DERIVATIVES VIA THREE-COMPONENT ONE-POT REACTION.

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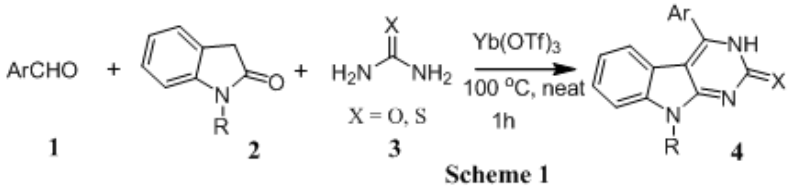
Indole nucleus is a prominent structural subunit present in numerous natural products and synthetic compounds with vital medicinal value.[1] The poly cyclic annulated indole compounds continue to be of extensive synthetic interest, partly because there are many biologically active natural products of this type, and also because the polycyclic frameworks lead to relatively rigid structures that might be expected to show substantial selectivity in their interactions with enzymes or receptors.[2]

Multi-component reactions (MCRs) are powerful tools in modern medicinal chemistry, enabling straightforward access to large libraries of structurally related, drug-like compounds and thereby facilitating the generation of lead candidates compounds. Hence, combined with the use of combinatorial chemistry and high throughput parallel synthesis, such reactions have constituted an increasingly valuable approach to drug discovery efforts in recent years. [3],[4] Pyrimidinone skeleton exists in many natural or synthetic biologically active materials, and its derivatives are applied in various pharmaceutical and biochemical fields.[5],[6] Thus the development of facile synthetic methods towards pyrimidin-2(1H)-ones, constitutes an active area of investigation in organic synthesis. Lewis acid reactions have attracted tremendous interest throughout scientific communities due to their low toxicity, ease of handling, low cost, stability, and recoverability of the reagent from water.[7] As part of our continued interest on indole and synthesis of diverse heterocyclic compounds of biological significance,[8] recently we reported an efficient method for the synthesis of α-carbolines from oxindole by exploring a 'three-component reaction in one pot'.[9] In the present paper, we report the synthesis of some novel pyrimido[4,5-*b*]indole derivatives from oxindole **1** via a three-component one-pot reaction using yitterbium(III) triflate as catalyst.



Scheme 1

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ALOVERA BASED PRODRUGS: PREPARATION AND DRUG RELEASE STUDIES

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Prodrugs of Alovera conjugated with nonsteroidal anti-inflammatory drugs such as Ibuprofen and Aspirin were prepared. The drug content of the prodrugs ranged from 18 to 48%.These prodrugs were characterized by IR and ^{1}H-NMR spectroscopy. The release rate of drugs was studied in-vitro at pH 1.2 and 7.4 spectrophotometrically in presence and in absence of enzymes. The release was much slower regardless of the presence or absence of enzymes at pH 1.2 (less than 15% in 6 h) for all the prodrugs of ibuprofen and aspirin. At pH 7.4 less than 15% of drug was released in 6 h in absence of enzymes for all the Prodrugs of ibuprofen and aspirin. In the presence of enzymes and in case of prodrugs of ibuprofen 37 to 60% of drug was released, while in case of prodrugs of aspirin 34 to 55% of drug was released in 6 h. The release rate was seen to decrease with increase in drug content.

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SYNTHESIS AND PROPERTIES OF ZnSe THIN FILMS GROWN UNDER REDUCING ATMOSPHERE.

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Being a promising and potential candidate of high performance in photovoltaic and optoelectronic applications, zinc selenide thin films with different Zn/Se ratios (0.571 to 0.993) were grown chemically onto glass substrates. The growth temperature (70 ^{0}C), time (210 min.), pH (10.5± 0.2) and quantity of hydrazine hydrate were optimized so as to obtain good quality films. The final product ZnSe films are physically hard, tightly adherent, relatively uniform and diffusely reflecting with light brown coloured tinge in smoky appearance. An EDS analysis showed that film stoichiometry depends on quantity of added reducing agent in the bath. As –deposited ZnSe is hexagonal wurtzite with <101> preferred orientation. The crystallite size decreased with decrease in Zn/Se ratio. The multifold roles of hydrazine hydrate (reducing and complexing agent, shape controller, stabilizing agent) have been examined through the FTIR studies. The 3343 cm^{-1} broad band for hydrazine hydrate can be assigned to asymmetric stretching vibrations of N-H group. For ZnSe, an upward shift (3353-3398 cm^{-1}) is observed and the band at 1615 cm^{-1} with a weak shoulder at 1578 cm^{-1} is observed due to the H-N-H symmetric and antisymmetric bending vibrations, respectively. After interaction with surface ions of ZnSe, the former band shows down shift whereas latter shoulder band disappeared. The changes in position of bands for ZnSe from 1423 to 1491 cm^{-1} (due to O-H bending) and 1343 cm^{-1} to 1369 cm^{-1} (due to N-H bending) have also been observed. ZnSe showed direct type of transitions with an optical gap decreased from 2.71 eV to 2.60 eV when Zn/Se ratio is increased from 0.993 to 0.571. AFM studies revealed changes in surface roughness, RMS values and average height with change in Zn/Se ratio.

PP 93

SYNTHESIS AND CHARACTERIZATION OF NANO METAL COMPLEXES OF 1,2 NAPHTHOQUINONE OXIMES AND STUDY OF THEIR ANTIMICROBIAL ACTIVITIES

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Metal complexes of 1,4 and 1,2 naphthoquinone based ligands especially their oxime derivatives are of special interest. Several of these metal complexes are found to possess extremely tiny particle size of the order of 10-90 nm. This was firstly observed while filtering the precipitate of some lanthaninde chelates of 1,2 and 1,4 naphthoquinone oximes. These chelates were found to pass through Whatman filter paper 41 or 42 indicating that their particle size is extremely small. Therefore, the XRD patterns of these lanthanide oximates were recorded whose nature clearly indicated the possibility of their nanometric nature. Their SEM photography also provided supporting evidence for nanoscale particles. The particle size determination through XRD pattern using Scherer equation (10-90 nm) confirmed that, these oximates are nanochelates. Subsequently many other metal chelates of 1,2 an 1,4 naphthoquinone based ligands were found to follow similar trends.

These significant findings are promising to develop science and technology of nanometal complexes as a new branch which may be recognized as **nanocoordination chemistry.** From this point of view we are trying to synthesise more and more nanoscaled metal complexes and characterize their nanometric nature through XRD and SEM along with their chemical and structural aspects using instrumental techniques like EDX, XPS, TG/DTG, IR and UV spectroscopy.

In this communication, we would like to report our recent work on synthesis and characterization of some 1,2 napthoquinone metal oximates along with the study of their antimicrobial activities. The selected ligands include isomeric 1,2 naphthoquinone monoximes while the selected metals include Fe (II), Ni (II), Nd (III) and Gd (III).

The metal complexes are synthesized by using the methods established in our laboratory and these are characterized through chemical analysis and TG/DTG. Their nanometric nature is confirmed with the help of XRD as well as SEM. The structural investigations are done by the use of IR and UV spectroscopy and magnetic susceptibility measurements. The antimicrobial activities are studied against two Gram positive, two Gram negative and one Fungal micro-organisms using well diffusion method.

The results of our investigations are examined to assess the effect of isomerism on various chemical, structural and antimicrobial properties.

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EFFECT OF CHELATION AND ISOMERISM ON ANTIMICROBIAL ACTIVITY OF COPPER(II) CHELATES OF ISOMERIC JUGLONES

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Isomeric Juglones are hydroxyl derivatives of 1, 4 naphthoquinones which possess powerful chelating ability. During the structural investigations of metal juglonates based on XRD and SEM, it was found that the crystallite size of many of these juglonates lies in the range of (10-100) nm suggesting their nanometric nature. This exciting observation is indicative of the possibility of developing a new branch which may be recognized as Nano Coordination Chemistry under which a series of Nano metal chelates may be synthesized. Their nanometric nature may be explained and confirmed with the help of XRD, SEM and TEM. Detail studies of these nanochelates from chemical, structural and biological points of views are expected to make some significant contributions to the field of coordination chemistry. Our present attempts are in these directions.

In this communication, we would like to report the synthesis and characterization of the copper (II) Nano Chelates with isomeric juglones, Lawsone-Juglone and Phthiocol-Plumbagin and study of their antimicrobial activities.

The chelates are synthesized using literature methods whose chemical identities are established through elemental analysis and TG. Their nanometric nature is identified with the help of XRD and SEM. The antimicrobial activities are examined at neutral pH against Micrococcus luteus, Klebsiella pneumonia and Asperillus flavus using well diffusion assay method.

Results of these investigations are employed to asses the effect of chelation and isomerism on the antimicrobial activities with special reference to the nanometric structure of these chelates.

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APPLICATION OF THE TECHNIQUE OF BHASMIKARNA TO SYNTHESIZE NANOMERIC CARBON BASED AYURVEDIC DRUG : HIRAKA BHASMA

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Nanopharmaceuticals and nanodrugs constitute an important class of nanomaterials of medicinal importance. The exponentially enhanced medicinal potency of a nanodrug or nanomedicine is now well established in modern pharmaceutical sciences as well as other traditional medicinal systems. Among these, ayurved is most ancient medicinal system of Indian origin.

In Ayurvedic system of medicine, drugs of mineral origin are of special importance for research scientists. Carbon-based drug synthesized from natural diamond known as *hiraka bhasma* is one of such traditional drug. Genuine *hiraka bhasma* is claimed to be an excellent remedy for heart troubles, which stops severe heart pains, stimulates heart functioning and impart energy to dilated heart. It works effectively in contraction of veins, blood clotting and improves blood circulation. It is also a powerful tonic and antitumor agent.

The details of the synthesis of *hiraka bhasma* from diamond are described in ancient ayurvedic literature. The major steps of this synthesis consists of (i) choice of the appropriate sample of natural diamond. (ii) a specific operation called as ayurvedic purification (*shuddhi*) through which the hard structure of diamond is destroyed which becomes convertable into microfined powder (iii) transformation of this purified state into bhasma state by fallowing the traditional ayurvedic process called as *bhasmikarana.* Miraculous medicinal properties are claimed to be manifested in the resulting bhasma state.

The process of *bhasmikarana*:- 10g of hiraka powder after its *shuddhi* is mixed with rose water and after preparing its homogeneous paste it is subjected to '*Gaja puta*'(underground heating using cow dung cakes). This process is repeated for 14 times. Then this processed powder is treated with *aloe vera juice* and again subjected to '*Gaja puta*'. This treatment with *aloe vera juice* followed by the application of '*Gaja puta*' is repeated 14 times. This *Hiraka Bhasma* is, red orange coloured microfine powder.

The XRD patterns were recorded on Phlillips X – Pert Pro Powder Diffractometer while SEM photographs and EDX were recorded on JEOL – 35M-5200 Scanning electron microscope. The SEM photographs and crystallite size determination using Scherer equation clearly indicate the nanoscale structure of *hiraka bhasma* of the order of 5.0 to 6.0 nm. The XPS and Visible Raman spectra of this sample ware also recorded which indicated that there is a compete conversion of diamond into graphite like (sp^2) form whose exact nature is yet to be explored.

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COMPARATIVE STUDY OF CALCIUM BASEDAYURVEDICDRUG KAPARDIKA BHASMA AND PURE CALCIUM CARBONATE

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Kapardika Bhasma is one of the important calcium based ayurvedic drug of marine origin. It is prepared from naturally occurring *Karardika (Varatika)* by following traditional process of *Bhasmikarana*. This traditional ayurvedic process involves three major steps (i) Selection of an appropriate sample of *Kapardika* according to directions given in Ayurvedic literature and its purification called as *Shuddhi*. (ii) Conversion of this purified material into finely powdered state. (iii) Transformation of this powder into final *Bhasma* state by following ayurvedic process of *Bhasmikaran*a.

Excellent medicinal properties are ascribed to a genuine *Kapardika Bhasma* which include (i) antacid behavior (ii) Skin Infection especially Skin burning. (iii) chronic loss of apatite and (iv) Stomach ache induced after the meals (called as *parinamashula*).

From chemical point of view, *Kapardika Bhasma* is predominantly composed of calcium carbonate (95%) as its major constituent along with magnesium and Silica as the minor constituents (2-3%) and a number of trace constituents. Apart from these it is expected that organic component, which is invariably present in the original sample of *Kapardika*, should be present whose presence and important role is totally neglected up-till now.

All these properties are quite different than pure calcium carbonate and cannot be attributable to other minor or trace constituents alone. Therefore, a comparative study of *Kapardika Bhasma* and pure calcium carbonate is carried out with a specific objective to search the factors which are behind the differential behavior of and the characteristic medicinal properties of *Kapardika* Bhasma.

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COMPARATIVE STUDY OF KINETICS OF REMOVAL OF FUCHSIN BASIC FROM AQUEOUS SOLUTIONS USING BIOSORBENTS

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Adsorption studies of Fuchsin basic (FB) on six different agricultural wastes / natural materials were carried out by batch experiments. The parameters studied include initial dye concentration, adsorbent dose, pH, agitation time, agitation speed, particle size of adsorbent and temperature. Freundlich, Langmuir and Temkin isotherm models were used to test the equilibrium data. The linear regression coefficient R^2 was used to elucidate the best fitting isotherm model. The best fitting isotherm models were found to be Langmuir ($R^2 \geq 0.997$) and Temkin ($R^2 \geq 0.992$). Freundlich isotherm was also found to be fit good enough with R^2 = 0.976 to 0.989 and n = 2.857 to 4.525. The monolayer (maximum) adsorption capacities (q_m) were found between 166.667 to 250 mg/g for adsorbents under study. Lagergen pseudo –first order model, Lagergen pseudo -second order model, Natrajan and Khalaf model, Bhattacharya and Venkobachar models were tested for the kinetic study. Lagergen pseudo -second order model best fits the kinetics of adsorption. The correlation coefficient R^2 for second order adsorption model has very high values for all adsorbents ($R^2 \geq 0.999$) and $q_{e(the)}$ values are consistent with $q_{e(exp)}$ showed that pseudo second order adsorption equation of Langergen fit well with whole range of contact time. Intra particle diffusion plot showed boundary layer effect and larger intercepts indicates greater contribution of surface sorption in rate determining step. Adsorption was found to increase on increasing pH, increasing temperature, increasing agitation speed and decreasing particle size. Thermodynamic analysis showed negative values of ΔG indicating adsorption was favourable and spontaneous, small positive values of ΔH below 40 KJ/mole indicating endothermic physical adsorption and positive values of ΔS indicating increased disorder and randomness at the solid-solution interface of FB with biosorbents. Adsorption capacity of pineapple peel powder towards FB was found to be more than other adsorbents under study**.**

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SYNTHESIS AND CYTOTOXIC ACTIVITY OF SOME IMIDAZO[2,1-B]-1,3,4-THIADIAZOLE DERIVATIVES

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Cancer is a disease characterized by uncontrolled growth of abnormal cells in the body. Anand et al. [1]. Development of anticancer drugs with fewer or no side effects is important for the treatment of cancer. a series of 2,5,6-trisubstituted imidazo[2,1-b]-1,3,4-thiadiazole derivatives have been synthesized by reacting 2-amino-1,3,4-thiadiazole and an appropriate 4-substituted /unsubstituted phenacyl bromide. Karki et al. [2]. Further 5-bromo, 5-thiocynato, 5-formyl derivatives were synthesized to study the effect on biological activity. Structures were established by IR, ^{1}H NMR, and mass spectras. The selected compounds were evaluated for their preliminary cytotoxic activity against murine leukemia cells (L1210/0), human T-lymphocyte cells (CEM) and human cervix carcinoma cells (HeLa). Karki et al. [3]. The results showed that SKS-47 [2-(4-chorobenzyl)-6-(2-oxo-2H-chromen-3-yl)imidazo[2,1-b][1,3,4]thiadiazole-5-carbaldehyde] exhibited more potent cytotoxicity (0.75 to 0.90µM) in comparison with standard Melphalan (2.1 to 3.2µM. Further study is under progress to understand its mode of action and *in-vivo* anticancer activity in our laboratory.

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SYNTHESIS AND CYTOTOXIC EVALUATION OF SOME STILBENE DERIVATIVES AGAINST MURINE AND HUMAN TUMOR CELLS

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Cancer is one of the major reasons of death in both men and women. One promising natural product is resveratrol (3,4',5-trihydroxy-*trans*-stilbene) a phytoalexin found in grapes and in red wine. The interest in this molecule has considerably increased in the last 10–12 years. The anticancer activity of resveratrol was first revealed by its ability to reduce the incidence of carcinogen-induced development of cancers in experimental animals. Jang et al. [1], Dong et al. [2]. We performed isosteric modification of resveratrol by keeping stilbene backbone of resveratrol. A series of stilbene derivatives have been synthesized by reacting substituted benzyl chloride, triphenyl phosphine to get phosphonium chloride which further reacts with sodium hydride, aryl aldehyde to form mixtures of stilbenes (*cis/trans* isomer) at 0-5°C, *trans*-stilbene separated by preparative TLC. Structures of these compounds were established by IR, ^{1}H NMR, mass spectras. The selected compounds were evaluated for their preliminary cytotoxic activity against murine leukemia cells (L1210/0) and human T-lymphocyte cells (Molt4/C8, CEM/0). The results showed that SS-28 {1,2,3-trimethoxy-5-[2-(4-methylphenyl)-ethenyl]benzene} exhibited more potent cytotoxicity (1.2 to 3.1µM) in comparison with standard Melphalan (2.1 to 3.2µM). Karki et al. [3]. Further study is under progress to understand its mode of action and *in-vivo* activity in our laboratory.

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PP 100

DE NOVO DESIGN, SYNTHESIS, SPECTROSCOPIC CHARACTERIZATION AND DNA-BINDING STUDIES OF NEW SULFASALAZINE–DERIVED DIPEPTIDE Zn(II) COMPLEX: VALIDATION FOR SPECIfiC RECOGNITION WITH NUCLEOTIDES AND DNA CLEAVAGE STUDIES.

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New water soluble complex [Zn(glygly)(ssz)(H_2O)]. $6H_2O$ **(1)** derived from dipeptide (glycyl glycine anion) and sulfasalazine was synthesized and characterized by spectroscopic (IR, UV-vis, NMR, ESI-MS) and analytical methods. The *in vitro* DNA binding studies of complex **1** with calf–thymus DNA were carried out by employing various biophysical methods and molecular docking technique which reveals strong electrostatic binding via phosphate backbone of DNA helix, in addition partial intercalation. To gain further insight into the molecular recognition at the target site, interaction studies of complex **1** with nucleotides (5′-TMP and 5′-GMP) were carried out by UV–vis titrations which implicate the preferential selectivity of complex **1** to N3 of thymine rather than N7 of guanine. Complex **1** exhibits a remarkable DNA cleavage activity (concentration dependent) with pBR322 DNA and cleaves via hydrolytic mechanism which was further evidenced by T4 ligase assay.

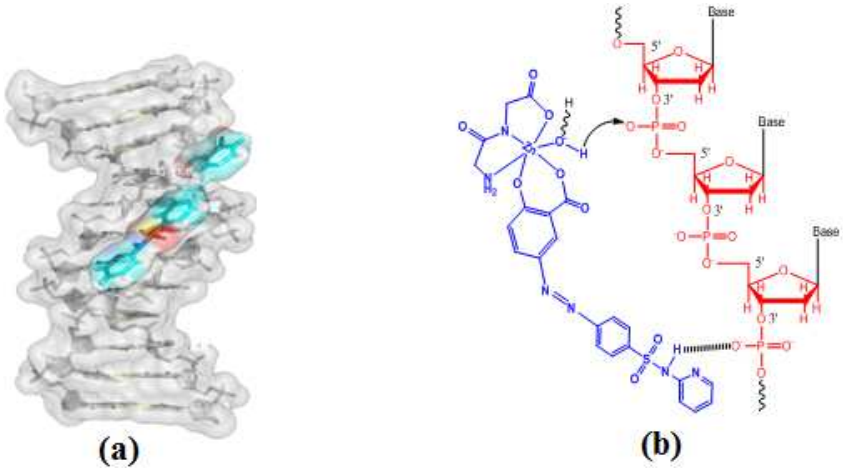

Fig: (a) Molecular docked model of complex 1 with DNA dodecamer duplex of sequence d(CGCGAATTCGCG)$_2$ (PDB ID: 1BNA) in the minor groove (b) Proposed intermediate in the hydrolysis of DNA cleavage promoted by heterobimetallic complex 1

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ANTIFUNGAL ACTIVITY OF AZOLE DERIVATIVES AND THEIR STRUCTURE–ACTIVITY RELATIONSHIPS

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In recent years series attention has been directed toward the discovery and development of new antifungal drugs. Mostly caused by Candida albicans, these infections are often spread through the use of broad-spectrum of antibiotics agents, anticancer, and anti-AIDS drugs. Azoles derivatives are present in many effective antifungal drugs, widely used for the treatment of topical or inner mycoses, in particular AIDS-related mycotic pathologies. Bearing in mind the above observation, we were synthesized various azole derivatives and characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, mass spectral studies and some of compounds characterized by X-Ray crystallography analysis. The compounds were assayed for their *in vitro* broad-spectrum antifungal activity, compared to clotrimazole and fluconazole, against 20 clinical isolates of pathogenic Candida spp., representing five different species. The results showed that the presence of azole revealed heterocyclic or bicyclic rings promising selective inhibitory activity especially against Candida albicans and Candida glabrata. To investigate the antifungal data on structural basis, molecular modeling, structural activity relationship and docking studies of proposed binding mode of novel azole derivatives as enzyme inhibitors.

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SYNTHESIS AND CHARACTERIZATION OF MESOPOROUS MATERIALS FROM CTPS-FLY ASH AND AMORPHOUS SILICA FROM RICE HUSK ASH

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Two methods have been evaluated for the synthesis of mesomorphous material zeolites using fly ash from Chandrapur Thermal Power Plant and amorphous silica from rice husk ash as raw materials. One consists of a hydrothermal process in which fly ash and amorphous silica from rice husk ash were mixed with a sodium hydroxide solution at 120 ºC for 7 h. The other comprises a combination of the alkaline fusion of fly ash and amorphous silica from rice husk ash with sodium hydroxide prior to incubation. The fusion products were mixed with 100 ml distilled water. The fusion methods have been evaluated at different proportions of fly ash and amorphous silica/sodium hydroxide in order to optimize the synthesis. Hydrothermal process gave the product of unnamed zeolite and low CEC value. Alternatively, in the fusion method, the fly ash and amorphous silica ratio of 7:3 showed that Na-x hydrate zeolite (FAU) is the main phase of the products. The infrared spectra showed the strong band near 1000 cm-1 which are both Si-O-Si and Si-OAl asymmetric stretching modes. Furthermore, SEM indicated that the octahedral crystal of Na-x hydrate zeolite was 360 meq/100g.

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SYNTHESIS OF *MESO*-FUNCTIONALIZED PORPHYRINS: THEIR DNA BINDING AND PHOTOCLEAVAGE STUDIES

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Porphyrins have been widely studied in a variety of applications in the fields of materials chemistry, nanotechnology, biosensors, fluorescence imaging, catalysis and medicine particularly, photodynamic therapy (PDT). [1] Appreciable progress has been made to develop new synthetic protocols to prepare modified porphyrins for the production of functionalised arrays or tune the physico-chemical properties favourably for intended medicinal or electronic applications.[2-5] Introduction of functional groups on porphyrins has been done either by condensation of funtionalized aldehydes or by modifications of preformed porphyrin at *meso*□ or □□□positions to obtain unsymmetrically substituted porphyrins intended for various applications.[6] In our on-going efforts to prepare novel functionalized porphyrins [7, 8] we have synthesized 5-(4-cyanophenyl)porphyrin from porphyrin thioamide by using hypervalent iodine reagent and studied their behavior in presence of calf thymus DNA using UV-vis and fluorescent spectroscopies. Absorption spectra of these porphyrins showed significant shift of the soret band in presence of CT DNA. In emission studies we found marked increase in fluorescence with increasing concentration of CT DNA. The cationic 5-(4-cyanophenyl)-10,15,20-tripyridylporphyrin showed efficient photocytotoxicity at 1.0 μM concentration against ΦX1104 plasmid DNA. Details about synthesis, characterization and biological studies of 5-(4-cyanophenyl)porphyrins will be discussed in the poster presentation.

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SYNTHESIS AND DNA INTERACTION STUDIES OF PORPHYRIN APPENDED THIAZOLES

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The search for novel tetrapyrrolic macrocycles with particular features for specific applications (e.g., photodynamic therapy (PDT) of cancer, catalysis, electronics, solar-cell production, etc.) has become a target for several research groups [1]. Researchers have contributed extensively to the development of porphyrin based heterocycles and used them in the construction of a range of porphyrin-based supramolecular assemblies [2]. In the past, various strategies were explored towards macromolecular modification [3], 1,3-dipolar cycloaddition and electrocyclization reactions in the development and improvisation of synthesis for novel porphyrins [4]. In order to mimic porphyrins selectively into biological systems and tune their optical and redox properties for different applications, efficient methods for functionalizing the porphyrin core are constantly under investigation [5]. On the other hand, alkynyliodonium salts represent an interesting class of compounds in organic synthesis and used as a stable and readily available powerful alkynylating reagents. Extensive studies were carried out in the preparation, structure and reactivity patterns of alkynyl(aryl)iodonium [6]. Synthesis of various thiazoles was known on reacting thiamide with alkynyl(aryl)iodonium tosylate [7]. In continuation to our efforts in synthesis of novel porphyrin appended heterocycles [8] we have synthesized various novel porphyrinthiazoles from the reaction of appropriate porphyrin thiamide with alkynyl(aryl)iodonium tosylates. Detail synthesis and DNA interaction studies of novel porphyrinthiazoles will be discussed in the presentation.

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LIQUID CHROMATOGRAPHY/TANDEM MASS SPECTROMETRY FOR THE SIMULTANEOUS DETERMINATION OF ALVERINE AND ITS METABOLITE, MONOHYDROXY ALVERINE, IN HUMAN PLASMA: APPLICATION TO A PHARMACOKINETIC STUDY

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A rapid and sensitive LC-MS-MS method for the determination of alverine (ALV) and its major metabolite, monohydroxy alverine (MHA), in human plasma using imipramine as an internal standard was developed and validated. The analytes were extracted from 0.5 mL aliquots of human plasma by solid phase extraction, using oasis cartridge. Chromatographic separation was carried on Thermo Gold C18 column (50 x 4.6 mm, 5 μ) at 30 °C, with isocratic mobile phase, a flow rate of 0.4 mL/min and a total run time of 3.5 min. Detection and quantification were performed using a mass spectrometer in the selected reaction-monitoring mode with positive electrospray ionization at *m/z* 282.3 - 91.11 for alverine, *m/z* 298.3 - 106.9 for mono-hydroxy-alverine, and *m/z* 281.0 - 86.0 for internal standard (IS) respectively. This assay was linear over a concentration range of 0.060-10 ng/mL with a lower limit of quantification of 0.060 ng/mL for both alverine and monohydroxy alverine. The coefficient of variation for the assay precision were <9.18% and <8.44%, the accuracy were >104.66% and >100.38% for alverine and monohydroxy alverine respectively. This method was successfully applied to a pharmacokinetic study after oral administration of alverine citrate 60 mg capsule in healthy male subjects.

PP 106

ARYLATION OF UNPROTECTED QUINOLINE DERIVATIVES USING SUZUKI MIYAURA REACTION IN WATER

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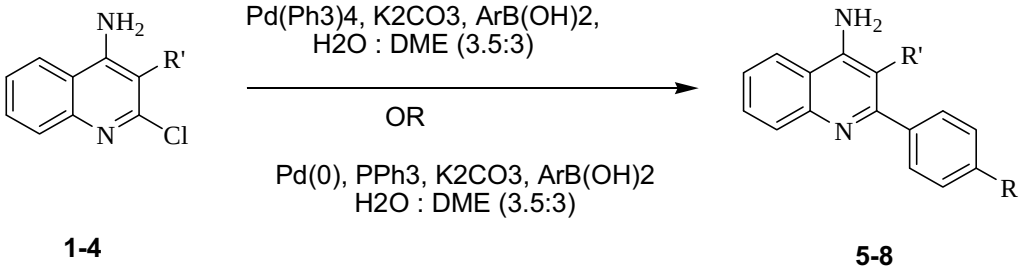
In year 2010 Nobel Prize in Chemistry was awarded to Richard F. Heck, Ei-ichi Negishi and Akira Suzuki for their contribution in development of palladium-catalyzed cross coupling. This chemical tool has vastly improved the possibilities for chemists to create carbon-based molecules as complex as those created by nature itself. Carbon-carbon bond formation in diversely functionalized 4-amino-2-chloroquinolone derivatives was done using Suzuki-Miyaura cross coupling in aqueous medium. Parallel experimentation proved efficiency of tetrakistriphenylphosphine palladium catalyst over other catalyst using weak nucleophiles arylboronic acid. The optimum conditions are tetrakistriphenylphosphine palladium catalyst; water and DME as co-solvent, reaction time 8 hour and need of electron deficient substitution at C_3 for efficient arylation of 4-amino-2-chloroquinolone derivatives.



1-4 **5-8**

R= -COOEt; COOH; CH2OH; CHO

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PP 107

SYNTHETIC LIBRARY OF CYCLOHEXANE-DIAMINE DERIVATIVES AS POTENTIAL ANTIMICROBIAL AGENTS

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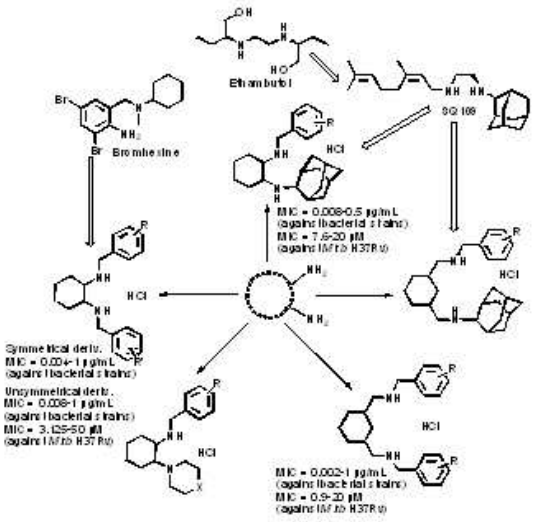
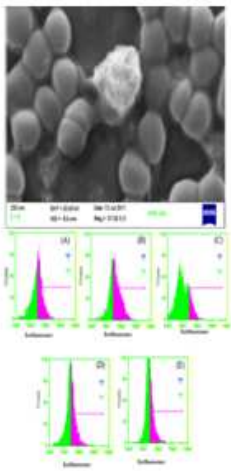
Bacteria have been the cause of some of the most deadly diseases and widespread epidemics of human civilization. Bacterial diseases such as tuberculosis, typhoid fever, cholera, dysentery, pneumonia, typhus, plague and diphtheria have taken a mighty toll on humanity. Tuberculosis is a contagious, deadly disease which spreads through air and caused by various strains of mycobacteria, these includes *Mycobacterium tuberculosis*, *M. africanum* and *M. avium* [1, 2]. Presently, 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. The *N*-Alkyl benzylamine. bromohexine (mucolytic agent) isolated from Indian shrub *Adhatoda vasicca* shows pH-dependent growth inhibitory effect on *M. tb* [3]. As a part of our ongoing efforts towards the synthesis of novel antimicrobial agents, we became interested to modify the bromhexine molecule [4, 5]. A library of symmetrical and unsymmetrical cyclohexanediamine hydrochloride salts were synthesized and evaluated for their anti-tubercular as well as antibacterial efficacy [6, 7]. These compounds were found to have potent activity against *M. tb* H37Rv, Gram-negative and Gram-positive strains without any hemolysis [8].Most of the compounds also showed potent activity against methicillin resistant strain of *S. aureus* (MRSA). SEM and PI uptake experiments showed that cell wall might be the target of these compounds.





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PP 108

SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL STUDIES ON NEW SUBSTITUTED PYRAZOLINE DERIVATIVES.

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A new series of 2-substituted -1-(4-substituted)-3-substituted-4,5-dihydropyrazol-1-yl)ethanone are synthesized.Ortho and para substituted phenol is refluxed with ethylchloroacetate in dry acetone in presence of anhydrous potassium carbonate to yield ethyl (2,4-substitutedphenoxy) acetate(1). (1)On reaction with hydrazine hydrate yields 2-(2,4-substitutedphenoxy) acetohydrazide(2). Chalcones (3a-3j) are prepared from the reaction between substituted aldehydes and substituted acetophenones in presence of a strong base. (2)On reaction with chalcones afforded the pyrazoline derivatives. The structures of the compounds have been confirmed on the basis of ^{1}HNMR, IR and Mass spectral analysis. The compounds were screened for antibacterial and antifungal activities by cup-plate method as well as for anticancer activity.

PP 109

AN EFFICIENT SYNTHESIS OF 1,2,4-TRIAZIN DERIVATIVES AND THEIR IN VITRO ANTIMICROBIAL ACTIVITY

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A simple and efficient synthesis of 1,2,4-triazing derivatives is described by the condensation of substituted 4-(2-chloro-quinoline_yl methylene)-2-[Phenyl-4H-oxazol-5-one and phenyl hydrazine an equimolar sodium acetate and acetic acid as a solvent. The newly synthesized compounds were evaluated for their antimicrobial activity.

PP 110

NOVEL POLY(ETHER-AMIDE-AZOMETHINE)S: SYNTHESIS AND CHARACTERIZATION

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A novel aromatic diamine containing preformed aromatic –aliphatic amide and ether linkage, bis-[(4'-aminobenzyl)-4–benzamide] ether (BABE) was synthesized and characterized by FT-IR, ^{1}H, ^{13}C NMR and Mass Spectrometry. A series of new aromatic poly(ether-amide-azomethine)s was prepared by solution polycondensation of BABE with isomeric aromatic dialdehydes, namely isophthalaldehyde (IPA) and / or terephthaldehyde (TPA) in different mole % proportions. These polymers were characterized by FT-IR, viscosity measurement, solubility, TGA, DSC and XRD. The polymers had moderate molecular weights as evidenced by the inherent viscosities in the range 0.22 – 0.37 dL/g and these polymers dissolved in aprotic polar solvents containing LiCl. Polymers did not show any weight loss below 313 ^{0}C and retained 21 to 39 % weight at 900 ^{0}C (Char yield) when investigated by TGA under nitrogen atmosphere demonstrating good thermal stability. The DSC curves of poly(ether-amide-azomethine)s showed glass transition temperatures in the range of 202 to 238 ^{0}C. Wide angle X – ray diffraction (WXRD) analyses showed that the polymers were semicrystalline in nature.

PP 111

DPA MEDIATED EFFICIENT ONE POT SYNTHESIS OF TETRAHYDROBENZO(B)PYRANE DERIVATIVES IN AQUEOUS MEDIA

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A simple, efficient and environmentally friendly one pot protocol for synthesis of Tetrahydrobenzo (b) pyrane derivatives has been developed using DPA as catalyst. Cyclo-condunsation of 5,5dimethyl-1,3 cyclohexanedione, malenonitrile and aldehydes in distilled water offered the corresponding Tetrahydrobenzo(b)pyrane derivatives in good to excellent yield. Green solvent and easy work up procedure are the attractive features of this protocol.

PP 112

BIODEGRADATION OF CONGO RED DYE BY DRIED FUNGAL BIOMASS OF PUFFBALL (LYCOPERDON SP.)

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Fungal biomass has the ability for de-colorization and degradation of wide variety of dyes successfully through a number of mechanisms. A dried fungal biomass of puffball previously identified as *Lycoperdon* Sp., was used in the treatment of synthetic dyes effluent efficiently. In the present work, the synthetic azo dye Congo red was tested chemically with dried fungal biomass of puffball. The effect of pH, dye concentration, dried biomass was performed. After the bioremediation step, the complete biodegradation and decolarization are observed by UV-Visible spectrum and Fourier transfer infra red spectroscopy (FT-IR). The obtained data suggests that the dried biomass of fungus could be efficiently used for bioremediation of Congo red dye. Further microbial toxicity and phytotoxicity were also studied to assess the toxicity level for original dye and microbial treated decolorized products. The toxicity assessment result indicating the microbial treated decolorized products remarkably reduces the toxicity level of dyes. Therefore, puffball fungus could be used efficiently in the treatment of dyes industrial waste water without the risk of obtaining high carcinogenic or genotoxic compounds.

PP 113

ANTIHYPERGLYCAEMIC ACTIVITY OF SELECTED EDIBLE AND MEDICINAL PLANTS

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The antihyperglycaemic effect of crude powder, ethanolic and aqueous extracts of bulb of *Allium sativum* and *Allium cepa*, dry sap *of Aloe vera*, leaves of *Bauhinia forficata*, *Eucalyptus globules*, *Ipomea batatas*, and *Mangifera indica*, whole plant of *Catharanthus roseus*, and *Phyllanthus niruri*, seeds of *Caesalpinia bonducella*, roots of *Potentilla fulgens*, and hard wood of *Ficus bengalensis*, *Tinospora crispa*, and *Terminalia arjuna* were investigated in normal and streptozotocin (STZ) induced diabetic rats with and without sucrose [1, 2]. The improvement on oral glucose tolerance (OGTT) by crude powders of the above said ranged between 8.70 to 16.8 %, however ethanolic extracts of *A.sativum*, *A. cepa*, *C. bonducella*, *E.globules*, *P.niruri*, *P.fulgens*, and *T.crispa* exhibited improvement on OGTT to the order of 9.90, 17.0, 13.8, 15.3, 13.6, 15.1, and 20.6%, respectively and the aqueous extracts of *A.vera*, *B.forficata*, *C. roseus*, *F.bengalensis*, *M.indica*, *I.batatas* and *T .arjuna* showed improvement to the order of 9.14, 12.2, 9.78, 11.2, 14.1, 7.74, and 7.68 %, respectively on normoglycaemic rats. The ethanolic extracts of *A.sativum*, *A.cepa*, *C .bonducella*, and *T. crispa* showed decline in blood glucose levels to the tune of 17.3, 18.1, 19.0, and 15.6%, respectively, on STZ-induced diabetic rats without sucrose challenge and by 22.3, 30.8, 13.0, and 24.3%, respectively on STZ-induced diabetic rats with sucrose challenge. The aqueous extracts of *A.vera*, *B.forficata*, *F.bengalensis*, *I.batatas* and *T.arjuna* showed decline in blood glucose levels by 9.59, 12.2, 13.9, 20.3, and 12.2%, respectively on STZ-induced diabetic rats and 24.1, 25.1, 16.2, 15.6, and 16.2 %, respectively on STZ-induced diabetic rats with sucrose challenge. The antihyperglycemic extracts of the parts of these plants are being fractionated towards the search of the antidiabetic ingredients present in these.

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PP 114

SYNTHESIS OF 3-BROMOIMIDAZO[1,2-A]PYRIDINE DERIVATIVES VIA INSITU OXIDATION OF HBR BY NITRIC ACID

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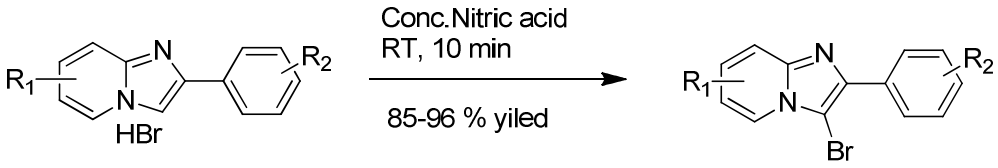
The imidazo[1,2-a]pyridine scaffold when functionalized appropriately is a starting point for preparation of a plethora of biologically active molecules. Appropriately functionalized imidazo[1,2-a]pyridine are also an attractive building block for the synthesis of tricyclic heterocycles. Herein an efficient, a novel synthesis of 3-bromoimidazo[1,2-a]pyridines is being reported with an excellent yields. The method involves insitu generation of HBr which is further utilized for bromination in presence of Nitric acid as an oxidant.



PP 115

APPARENT MOLAR VOLUME AND VISCOSITY B-COEFFICIENT OF POTASH ALUM IN WATER AND WATER + N, N-DMF MIXED SOLVENT AT DIFFERENT TEMPERATURES .

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Measurements of densities and viscosities of potash alum in water and water + (0 %, 5%, 10 %, 15 % and 20%) N,N-dimethylforamide have been made as function of molality at T = (298.15, 303.15, 308.15, and 313.15) K and at atmospheric pressure. Density data have been used to calculate the partial molar volumes of potash alum. Viscosity data have been analysed by using Jones-Dole.equation and B coefficients have been calculated. Partial molar volumes and B coefficients have been used to draw the conclusions regarding structure making or breaking behavior of potash alum.

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PP 116

ELECTROCHEMICAL CHARACTERIZATION OF THERMALLY OPTIMIZED ELECTRODEPOSITED FeO THIN FILMS FOR SUPERCAPACITOR

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In the recent year's growing demands for energy and power sources are stimulated a interest in electrochemical supercapacitor (ECs) having lot of application like digital communication, electrical vehicles, memory back-up devices etc. Electrochemical supercapacitors are two types. i) Electrochemical double layer capacitors (EDLC) ii) Pseudocapacitor

The electrodes of the supercapacitor are mainly prepared by carbon, transition metal oxides and conducting polymers. Various transition metal oxides are being studied for the supercapacitor application. Some are promising candidates for the supercapacitor application but are costly, toxic and less abundant. Iron oxide is the transition metal having low cost, can be prepared by various technique and found abundantly. Therefore in the present investigation by using well known electrodeposition technique thin films of FeOx were deposited onto stainless steel substrates using 0.1M aqueous solution of ferric chloride at different time periods. Prepared from 10 minutes to 60 minutes samples were annealed at a different temperatures from 3230 K to 6730 K by the interval of 500 K. Their structural and morphological study was carried out using XRD and SEM. To understand the conductive behavior of the prepared sample band gap for the typical sample was confirmed using UV optical study. In the capacitive studies electrochemical analysis was done to calculate specific capacitance (CS), specific energy (SE), specific power (SP) and columbic efficiency (ŋ) of the optimized sample. Also impedance study was carried to see the frequency behavior and internal resistance. Also the possible equivalent circuit is proposed.

PP 117

ELECTROCHEMICAL ANALYSIS OF MOLAR OPTIMIZED MnO FOR SUPERCAPACITOR

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Electrochemical capacitors are the energy storage devices which are having power and energy rating in the batteries and conventional dielectric capacitors. They have lot of applications like power supply, DC power systems, hybrid vehicles, Space vehicles etc. Depending on charge storage mechanism these are divided in to two types i) Double layer capacitor and ii) Pseudocapacitor.

Lot of transition metal oxides, carbons and polymers were tried in the preparation of electrode for supercapacitor. The most suitable transition metal oxides are found costly, hazardous and less abundant. Manganese oxide is one of the transition metal oxide showing well electrochemical behavior, of low cost and eco-friendly.

Therefore in the present investigation by using popular electrodeposition technique, thin films of MnO were deposited on to stainless steel substrates for 30 minutes. The molar variation of aqueous manganese acetate solution was from 0.02M to 0.01M by the interval of 0.01M. The prepared samples were annealed at the constant temperature 623^0K for 1 hour. The typical sample from this is again deposited for variable time periods from 10 minutes to 60 minutes. There structural and morphological study was carried out using XRD and SEM. The optical absorption was studied to understand the conductive nature of the prepared sample. In the Supercapacitive studies electrochemical behavior of the deposited sample was studied in 1M Na_2So_4 electrolyte using cyclic voltammetry to calculate capacitance (C), Specific capacitance (SC), and by using galvanostatic charge discharge to calculate specific energy (SE), specific power (SP) and coulomb efficiency (ŋ) . Also impedance study was carried to see the frequency behavior and internal resistance. Also the possible equivalent circuit is proposed.

PP 118

CHEMICAL DEPOSITION OF $Pb_{1-x}Hg_xS$ DETECTING THIN FILMS

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A liquid phase chemical bath deposition (LPCBD) for deposition of $Pb_{1-x}Hg_xS$ ($0 \leq x \leq 0.3$) thin films on glass microslides is presented. For deposition, triethanolamine complex of lead acetate and mercuric chloride were allowed to react with an aqueous thiourea solution. TEA slows down the precipitation action and facilitates deposition of Pb^{2+}, Hg^{2+} and S^{2-} in an alkaline medium. The film formation process is found to depend on the various preparative parameters / deposition conditions. These preparative parameters are optimized earlier and are used in these studies for monitoring the film deposition. The film growth takes place by an ion by ion condensation and is measured in terms of a layer thickness. The reaction mechanism and growth kinetics have been explored. The as-grown films appear smooth, tightly adherent, uniform and reflecting upto x=0.3 whereas, for higher compositions (x), the layer thickness continuously decreased. The colour of the deposits changed from blackish-grey to chocolate brown. The as-grown films were analyzed by an EDS technique for the contents of Pb, Hg and S. From the Pb/S ratio, it appeared that the PbS samples are stoichiometric at relatively higher values of pH. The observed average Pb : S ratio is 1.05 (at pH 10.5), which indicates that the product composition of Pb^{2+} and S^{2-} is at an approximate ratio of 1:1. The electrical behaviour was investigated for both PbS and $Pb_{1-x}Hg_xS$ films. The films have high electrical resistance ranging between 10^6 - $10^8\Omega$ and it increased with an increase of Hg content in the $Pb_{1-x}Hg_xS$ film.

PP 119

DEVELOPMENT OF SOLID-SELF MICRO EMULSIFYING FORMULATION BY SPRAY DRYING TO IMPROVE ORAL BIOAVAILABILITY

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Nearly 40% of new drug candidates exhibit low solubility in water, which leads to poor oral bioavailability, high intra- and inter-subject variability and lack of dose proportionality. One of the most popular and commercially viable formulation approaches for this challenge is Solid-self micro emulsifying drug delivery systems (S-SMEDDS). Gursoy R.N. et al. [1] The main objective of the study was to develop and evaluate an optimal S-SMEDDS formulation containing Hydrochlorothiazide (HTZ) by spray drying technique. In present study solubility of HTZ was determined in various oil, surfactant and co-surfactant. Pseudoternary phase diagrams were used to evaluate the microemulsification existence area. Three component SMEDDS formulation were established. Selected combinations were exposed to spray drying using water soluble maltodextrin as solid carrier. Bo Tang et al. [2]. S-SMEDDS formulations were tested for microemulsifying properties and for solid state characterization. The *in-vitro* dissolution studies of S-SMEDDS of HTZ filled into hard gelatin capsule and pure drug formulation was carried out. Results showed that the mean droplet size of all reconstituted S-SMEDDS were very low and all were found to be in the nanometric range (<100 nm). Drug releases from S- SMEDDS formulations were found to be significantly higher as compared with that of conventional HTZ tablet. Thus study concluded with S-SMEDDS provides useful solid dosage form to improve solubility and dissolution rate of HTZ and concomitantly bioavailability.

Fig. 1: Pseudo ternary phase diagram

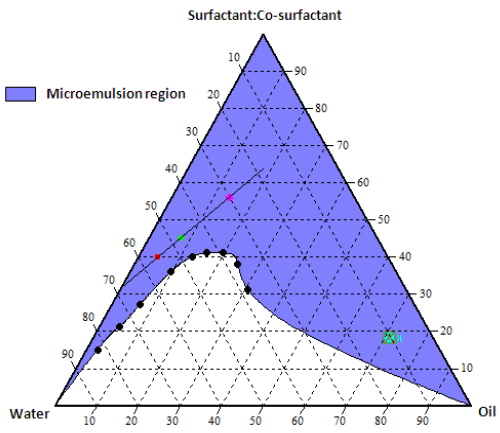
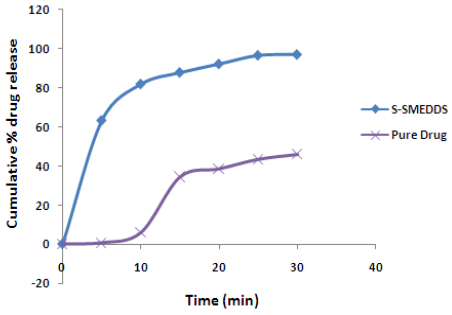


Fig. 2: *In-vitro* drug release of HTZ from S-SMEDDS compared with pure drug



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PP 120

3-PHENYLISOXAZOLE ANALOGS AS DGAT1 INHIBITORS: SYNTHESIS AND BIOLOGICAL EVALUATION

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Obesity, characterized by an accumulation of triglycerides in adipocytes, is a risk factor for hypertension, diabetes, and cardiovascular disease. Orlistat, the present therapeutic option for treatment of obesity is largely inadequate thereby presenting a pressing need for improved therapies that are more efficacious and give rise to fewer side effects. This has intensified research of newer mechanistic targets that seek to inhibit triglyceride biosynthesis and storage within the adipose tissue. Diacylglycerol acyltransferase, DGAT1, is a promising target enzyme due to its involvement in the final and only committed step of triglyceride biosynthesis. We have synthesized and evaluated 3-phenylisoxazole analogs as DGAT1 inhibitors. Several compounds within this novel scaffold exhibited potent DGAT1 inhibition when evaluated using an in vitro enzymatic assay that measures the formation of radioactive triglycerides. A few selected compounds from this series were also studied for their potential to reduce triglyceride levels in vivo using a fat tolerance test in mice. The synthesis and biological data of these 3-phenylisoxazole analogs will be presented.

PP 121

APPLICATION OF THE TECHNIQUE OF BHASMIKARNA TO SYNTHESIZE NANOMERIC CARBON BASED AYURVEDIC DRUG : HIRAKA BHASMA

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Nanopharmaceuticals and nanodrugs constitute an important class of nanomaterials of medicinal importance. The exponentially enhanced medicinal potency of a nanodrug or nanomedicine is now well established in modern pharmaceutical sciences as well as other traditional medicinal systems. Among these, ayurved is most ancient medicinal system of Indian origin.

In Ayurvedic system of medicine, drugs of mineral origin are of special importance for research scientists. Carbon-based drug synthesized from natural diamond known as *hiraka bhasma* is one of such traditional drug. Genuine *hiraka bhasma* is claimed to be an excellent remedy for heart troubles, which stops severe heart pains, stimulates heart functioning and impart energy to dilated heart. It works effectively in contraction of veins, blood clotting and improves blood circulation. It is also a powerful tonic and antitumor agent.

The details of the synthesis of *hiraka bhasma* from diamond are described in ancient ayurvedic literature. The major steps of this synthesis consists of (i) choice of the appropriate sample of natural diamond. (ii) a specific operation called as ayurvedic purification (*shuddhi*) through which the hard structure of diamond is destroyed which becomes convertable into microfined powder (iii) transformation of this purified state into bhasma state by fallowing the traditional ayurvedic process called as *bhasmikarana.* Miraculous medicinal properties are claimed to be manifested in the resulting bhasma state.

The process of *bhasmikarana*: 10g of hiraka powder after its *shuddhi* is mixed with rose water and after preparing its homogeneous paste it is subjected to '*Gaja puta*'(underground heating using cow dung cakes). This process is repeated for 14 times. Then this processed powder is treated with *aloe vera juice* and again subjected to '*Gaja puta*'. This treatment with *aloe vera juice* followed by the application of '*Gaja puta*' is repeated 14 times. This *Hiraka Bhasma* is, red orange coloured microfine powder.

The XRD patterns were recorded on Phlillips X – Pert Pro Powder Diffractometer while SEM photographs and EDX were recorded on JEOL – 35M-5200 Scanning electron microscope. The SEM photographs and crystallite size determination using Scherer equation clearly indicate the nanoscale structure of *hiraka bhasma* of the order of 5.0 to 6.0 nm. The XPS and Visible Raman spectra of this sample ware also recorded which indicated that there is a compete conversion of diamond into graphite like (sp^2) form whose exact nature is yet to be explored.

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SYNTHESIS OF BENZO[H][1,6]NAPHTHYRIDINES AS ANTIMALARIAL COMPOUNDS

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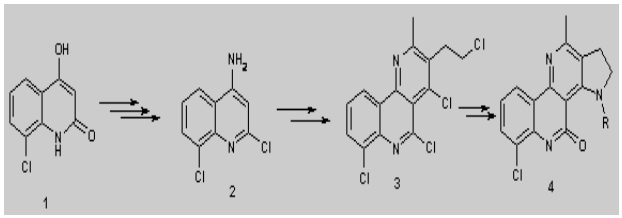
Synthesis of azido derivatives of hetarenes[1,2] raised question of regioselectivity during reactions of azide anion with 2,4-dichloroquinoline. 2,4-Dichloroquinolines are known to give nucleophilic substitution reactions both at□ □ and □-positions.[3,4] Kinetic studies of 2,4-dichloroquinoline indicate that the chloro atom at C_4 position is about two times more reactive towards nucleophiles[3,5] and predominantly an addition-elimination mechanism is observed[6]. In order to transform the literature findings for the introduction of azido groups, we have studied the reaction of 2,4,8-trichloroquinoline at different temperature. After reduction of 4-azido-2,8-dichloroquinoline with sodium dithionite gives required 2,8-dichloroquinolin-4-amine **2**. Number of electrophiles failed to react with weakly nucleophilic 4-amino group of the 4-aminoquinolines.[7] Utilization of the α-acetyl γ-butyrolactone was relatively strong electrophile provided us the route for synthesis of tricyclic and tetracyclic heteroaromatic compounds. As noted previously[8-9] several heterocycles with 2-chloroethyl side chain exhibited good in vitro activity against several cell lines of clinically isolated human tumor. Antimalarial candidates required the presence of a usable functional group at the 4-position of the tricyclic heteroaroaromatic nucleus. Since benzo[*h*][1,6]naphthyridin-4-chlorine possessed a requisite functionality, we sought a reaction which would provide this type intermediate in high yields. Reaction of 2,4,8-trichloroquinoline with sodium azide in DMF at 50°C leads to regioselective 4-azido 2,8-trichloroquinoline while the same reaction with excess of sodium azide in DMF at 80°C furnish 2,4-diazido 8-chloroquinoline in good yield. The 4-amino 2,8-dichloroquinoline **2** with □-acetyl-□-butyrolactone in toluene and PTSA furnished an intermediate dihydrofuranone at 120°C, which was further refluxed in $POCl_3$ give tricyclic 4,5,7 trichloro-3-(2-chloroethyl)-2-methyl benzo[*h*] [1,6] naphthyridine **3** at 130°C. The thermo selective nucleophilic substitution reactions of primary aromatic amine with compound **3** furnished 4,5,7-trichloro-3-(2-chloroethyl)-2-methylbenzo[*h*][1,6] naphthyridine at 110 °C while at 150°C gives pyrrolo [3, 2-*c*] benzo [*h*][1,6]naphthyridin-11-amine **4**. Similarly the regioselective substitution reaction of compound **3** with sodium azide in DMF at C_4 and also at aliphatic 3-(2-chloroethyl) side chain afford 4-azido-3-(2-azidoethyl)-5,7-dichloro-2-methylbenzo [*h*][1,6] naphthyridine and with sodium alkoxide in alcohol gives reaction at C_4 position afford 5,7-dichloro-3-(2-chloroethyl)-4-alkoxy-2-ethylbenzo[*h*][1,6]naphthyridine.



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PP 123

ASYMMETRIC SYNTHESIS OF MORPHOLINE DERIVATIVE LINEZOLID AND PIPERAZINE DERIVATIVE EPERZOLID

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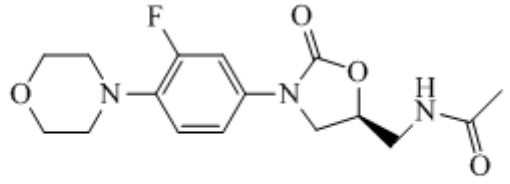
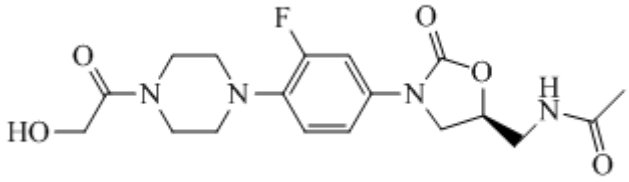
The 3-aryl-2-oxazolidinones are known to be new class of synthetic antibacterial agents which posses a new mechanism of action for early inhibition of bacterial protein synthesis. This particular type of moieties is active against gram-positive organisms namely methicilin-resistant *Saphylococcus aureus, Staphylococcus epidermitis* and vancomycin-resistant *enterococci*.[1] The morpholine derivative linezolid (1), and the piperazine derivative eperezolid (2) are important representatives of this class. The asymmetric linezolid and eperezolid synthesized [2-4] either by a chiral pool approach or classical resolution of racemates.



Linezolid (1)



Eperzolid (2)

In our research group, a novel approach has been developed for the enantio-selective asymmetric synthesis of Linezolid and Eperzolid. All the synthesized intermediates, required for the Linezolid (1) and Eperzolid (2) synthesis were characterized by ^{1}H NMR, ^{13}C NMR, FTIR and the enantiomeric excess was determined by HPLC method. The details synthesis route for intermediates of the Linezolid **(1)** and Eperzolid **(2)** would be elaborated.

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PP 124

ETHANOMEDICINAL VALUE OF AILANTHUS EXCELSA WITH REFERENCE TO ITS MINERAL COMPOSITION

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One of the major difficulties in ethanobotanical study is insufficient scientific verification regarding mineral constituents in a particular medicinal plant. Major pharmaceutical companies are currently conducting extensive research on plant materials gathered from the rain forests and other places for their potential medicinal value. *Ailanthus excelsa* Roxb., which is commonly known as 'ardu' and found throughout the tropical and subtropical parts of india, especially in dry tracts of Gujarat, Punjab, Hariyana and the Deccan plateau. Minerals like Calcium, Magnesium, Sodium, Potassium, Iron, Nitrogen, Sulphur and Phosphorus are analyzed in the leaves of *A. excelsa*. Ash content in the leaves of *A. excelsa* was found to be 10.4gm in 100gm of sample. Moisture content in the leaves of this medicinal plant was noted to be 6.43%, where as its pH value was 7.47.

PP 125

ESTROGEN: ITS CARCINOGENICITY AND PREVENTIVE MEASURES

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Amongst several other estrogen dependent cancers, breast cancer, a leading pandemic, affects women with a wide age group Gruber, A. *et. al.* [1] & Riggs, B.L. *et. al.* [2]. It is most frequent site of cancer in women. There are approximately 2-2.5 million cases of cancer in the country at any given time. The two most common cancers in women viz. cancer of breast and cervix account for half of the cancer burden. In India, 50% of women with breast cancer and 70% of cervical cancers present themselves in late stages, III and IV. It is therefore imperative to find avenues for downsizing the disease Levenson, A.S. and Jordan, V.C. [3].

The successful treatment of this disease is limited by the fact that essentially all breast cancers become resistant to chemotherapy and endocrine therapy Esteva, F. J. *et. al.* [4] & Kamb, A. *et. al.* [5]

The presentation will highlight the importance of estrogens in biological system in particular female body and possible preventive measures for estrogen dependent cancers. Furthermore, structure activity relationship (SAR) related to selective estrogen receptor modulators (SERMs, synthetic estrogens) will be discussed to design newer SERMs for management of estrogen dependent cancers and related disorders.

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BIOTRANSFORMATION OF SIMPLE AROMATIC ESTERS BY WHOLE CELL MICROBIAL CULTURE OF BURKHOLDERIA CENOCEPACIA

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Whole cell microorganisms can be good source to conduct various biotransformations. Microorganisms use enzymes to transform many natural and synthetic organic compounds with regio and enantioselectively to respective products. Lipases and esterases are main groups of natural biocatalysts that promote ester bond cleavage and formation. Microorganisms belonging to the genus *Bacillus* showed esterase activity and good enantiomeric ratios for the resolution of phenylethanol derivatives ($E > 30$) Mantovani *et al* [1]. The hydrolysis of both ethyl phenylacetate and racemic ethyl 2-phenylpropionate (EPP) was carried out by *Aspergillus oryzae*. Hydrolysis reactions of esters were observed faster than esterification. The use of such biocatalysts seemed to significantly influence the hydrolysis equilibrium, thereby suggesting some unexpected, differentiated effect on reactants and products stabilization Torre *et al* [2]. In present experiment *Burkholderia cenocepacia* was isolated from rhizosphere Caballero- Mellado *et al* [3,4] of sugarcane as phosphate solubiliser. It also showed antifungal activity and plant growth promoting potential by indolacetic acid production. Enzymes from *Burkholderia cenocepacia* hydrolysed various aromatic esters to respective carboxylic acids. The characterization of the products was carried out by chromatographic methods.

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GLOBAL REGULATORY SCENARIO ON NEUTRACEUTICALS

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Nutraceutical is recognized as a linguistic combination of "nutrient" and "pharmaceutical", and is accepted as "any substance that may be considered a food or part of a food and provides medical or health benefits, including the prevention and treatment of disease." In the pharmaceutical development process, nutraceutical is a requirement to have clinical test results from animal tests and studies, for verification of the effects. On the other hand, in the case of nutrition, there was no verification method for foods in preventing diseases in the past. In recent years however, as food composition has been scientifically proven to cause lifestyle-related diseases, and has become a social issue. M. Prasad Palthur et al. [1].

The approach to regulating and marketing nutraceuticals is notably heterogeneous on the global level. This is largely due to the challenges in classifying these products, absence of a suitable regulatory category for these hybrid products, and varying views on what is considered sufficient scientific substantiation to conclude the functionality. Sumeet Gupta et al. [2]

Globally, the regulatory authorities are aware of changing needs of consumers and proactively protect consumers by amending existing laws to accommodate changes. All the leading nations have a different regulatory framework for nutraceuticals, but in India old laws such as Prevention of Food adulteration Act, 1954, which regulates packaged foods, still exist for manufacturers. The regulatory framework of nutraceuticals in India needs attention from the relevant authorities. Hence aim of this article to discuss global regulatory scenario of nutraceuticals.

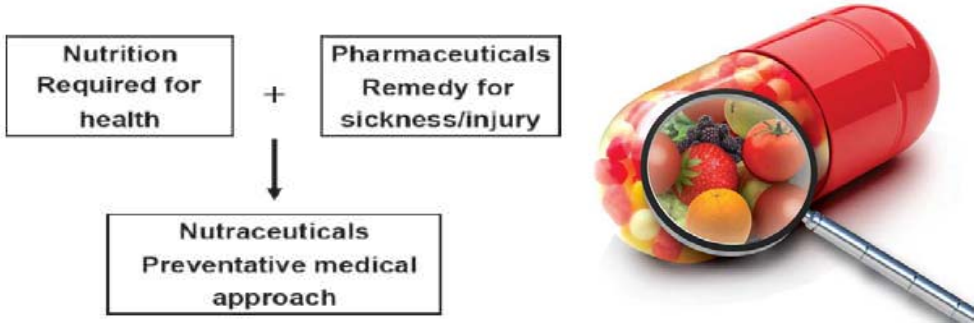

Figure 1: Concept of nutraceuticals

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PP 128

EFFECT OF CHELATION AND ISOMERISM ON ANTIMICROBIAL ACTIVITY OF COPPER(II) CHELATES OF ISOMERIC JUGLONES

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Isomeric Juglones are hydroxyl derivatives of 1, 4 naphthoquinone which possesses powerful chelating ability. During the structural investigations of metal juglonates based on XRD and SEM, it was found that the crystallite size of many of these juglonates lies in the range of (10-100) nm suggesting their nanometric nature. This exciting observation is indicative of the possibility of developing a new branch which may be recognized as Nano Coordination Chemistry under which a series of Nano metal chelates may be synthesized. Their nanometric nature may be explained and confirmed with the help of XRD, SEM and TEM. Detail studies of these nanochelates from chemical, structural and biological points of views are expected to make some significant contributions to the field of coordination chemistry. Our present attempts are in these directions.

In this communication, we would like to report the synthesis and characterization of the copper (II) Nano Chelates with isomeric juglones; Lawsone-Juglone and Phthiocol-Plumbagin and study of their antimicrobial activities.

The chelates are synthesized using literature methods whose chemical identities are established through elemental analysis and TG. Their nanometric nature is identified with the help of XRD and SEM. The antimicrobial activities are examined at neutral pH against *Micrococcus luteus*, *Klebsiella pneumonia* and *Asperillus flavus* using well diffusion assay method.

Results of these investigations are employed to asseses the effect of chelation and isomerism on the antimicrobial activities with special reference to the nanometric structure of these chelates.

PP 129

SYNTHETIC OPTIMIZATION AND BIOLOGICAL ACTIVITY OF PYRAZOLO-PYRIMIDINE CARBOXAMIDE BASED INHIBITORS

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Over the last decade protein kinases have poised themselves as valid targets for several anti-cancer therapeutic interventions[1]. Various novel heterocycles has been explored as receptor tyrosin kinase inhibitors. In recent past pyrazolo-pyrimidines have been explored as anti-cancer agents[2]. As a part of an ongoing medicinal chemistry program we explore pyrazolo-pyrimidine carboxamide as an anticancer agent. In this poster we report synthetic optimization and biological activity of pyrazolo-pyrimidine carboxamide based new chemical entities.

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PP 130

STIGMASTEROL AND β-SITOSTEROL: GLUCOAMYLASE INHIBITORS, ISOLATED FROM TULSI LEAVES.

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Glucoamylase inhibitors are oral antidiabetic drugs used for diabetes Type 2. They acts by preventing the digestion of carbohydrates. They are used to establish greater glycemic control over hyperglycemia. Acarbose and Miglitol are known glucomaylase inhibitors which reduces the impact of carbohydrates on blood sugar. In the present work, we have isolated Stigmasterol and β-sitosterol from ethanol extract of Tulsi leaves by column chromatography. These compounds showed remarkable inhibition of glucomylase activity *in vitro*. Thus, we report, first time isolation and characterization of Stigmasterol and β-sitosterol with 26.65% inhibition of glucoamylase. Hence stigmasterol and β-sitosterol together may control the blood glucose level when taken orally at very low concentration.

PP 131

ANTIOXIDANT, ANTIHYPERGLYCAEMIC AND ANTIDYSLIPIDEMIC ACTIVITY OF A-AMYRIN AND GINGEROL

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Diets rich in fructose produce glucose intolerance, obesity, insulin resistance, and dyslipidemia in animals. The high fuctose diet fed rats showed decreased PPARα mRNA and protein levels, suggesting that fructose or its metabolites can directly regulate lipid oxidation [1]. Considering this evidence, high fructose diet animal models were developed in the present study. It was observed that when HFD was fed to albino rats of Sprague Dawley strain developed mild hyperglycaemia and insulin resistance and Syrian golden hamsters developed dyslipidemia. Their serum triglycerides and cholesterol levels were increased and it was found 308.31±5.5mg/dl and 322.48 ±3.1mg/dl in comparision to normal diet fed animals having TG. 97.36±2.4 mg/dl and Chol.100.63±4.5 mg/dl after 8 weeks of feeding on this diet. High fructose diet fed rats were further given intra-peritoneal injection of streptozotocin at 30 mg/kg for rise in their blood glucose levels. After one week animals were tested for their blood glucose and their blood glucose was found 418.62±3.7 mg/dl in comparision to normal diet fed rats having blood glucose 69.5± 1.6. α-amyrin, and gingerol, the oleoresins from rhizhome of ginger have earlier been noticed for antihyperglycaemic and lipid lowering activity in db/db mice [2,3]. In the present study their antidyslipidemic activity has been confirmed in HFD fed Syrian golden hamsters and antihyperglycaemic and antioxidant activity in vitro. Antihyperglycaemic and antidyslipidemic activity has to further confirm in the above high fructose diet fed animal model.

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PP 132

SYNTHESIS AND PHARMACOLOGICAL EVALUATION OF NOVEL 4-THIAZOLIDINONE DERIVATIVES AS ANTIMICROBIAL AGENTS

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A series of novel 3-Ethyl-2-(3-fluoro-4-morpholin-4-yl-phenylimino)-5-(1H-indol-3-yl-methylene)-thiazolidin-4-one derivatives were synthesized for evaluation of their antibacterial and antifungal activity. The structures were determined by IR, NMR, mass spectroscopy and elemental analysis. They were screened for activities against bacterial and fungal strains. They exhibited moderate activities in screening in vitro studies.

Thiazolidinones are a class of important heterocyclics containing sulfur and nitrogen in a five member ring, and has been considered as a magic moiety (wonder nucleus) which posses almost all types of biological activities. This diversity in the biological response profile has also been receiving considerable attention of many researchers to explore this skeleton to its multiple potential against several activities. For instance, in recent years 4-Pheny-morpholine derivatives were reported to possess antimicrobial and anti-inflammatory activities. Thiazolidinones derivatives are also known to possess anti-bacterial, antifungal, antiviral and antituberculosis properties. Linezolide (commercially available antimicrobial drug) possess 4-(2-flouro-phenyl)-morpholine moiety, these observations led to the conception that Indole derivatives of 3-ethyl-2-(3-fluoro-4-morpholin-4-yl-phenylimino)-thiazolidin-4-one would possess potential antimicrobial properties.

In view of the broad spectrum of biological activities and the significant applications of Thiazolidinone ring system, we thought it was worthwhile to explore the synthesis and evaluation of various biological activities of novel Thiazolidinone derivatives. In the present study, we report an efficient synthesis of different Thiazolidinone derivatives using previously reported methods and prepared compounds screened for in-vitro antibacterial, anti-fungal activity, and the structure of the synthesized compounds were elucidated by ^{1}HNMR and EI-mass spectral data.

The present study showed that all the title compounds were exhibiting significant antibacterial and antifungal activities. However, further studies are required to establish the mechanism of action of the title compounds. From the screening data it was found that 4-methoxyphenylsulfonyl derivative have encouraging antibacterial and antifungal activity which need to be further investigated to get better agents.

PP 133

IN-VITRO ANTHELMINTIC ACTIVITY OF HOLARRHENA ANTIDYSENTERICA BARK

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Medicinal plants have served through ages, as a constant source of medicaments for the exposure of a variety of diseases. The history of herbal medicine is almost as old as human civilization.Today; the principal mode for control of gastrointestinal parasites is based on the commercial anthelmintic. Development of anthelmintic resistance and high cost of conventional anthelmintic drugs led to the evaluation of medicinal plants has an alternative source of anthelmintics. In the current study, in-vitro experiments were conducted to evaluate the possible anthelmintic effects of Bark of *Holarrhena antidysenterica* using Pheretima Posthuma Three concentrations (25, 50 and 100 mg/ml) of each extracts were studied in the activity, which involved the determination of time of paralysis and time of death of the worm. Piperazine citrate in same concentration as that of extract was included as standard reference and normal saline as control. The result of the present study indicated that both alcoholic and aqueous extract exhibited moderate to significant anthelmintic activity. The results demonstrated paralysis and also caused death of worms especially at higher concentration of 100 mg/ml, as compared to standard reference Piperazine citrate.

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PP 134

ROLE AND FUTURE OF CHEMISTRY AND BIOLOGY IN DRUG RESEARCH

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[$Cu(L_1)(Phen)(Cl)$],[$Cu(L_1)(Bipy)(Cl)$] and [$Ni(L_1)(Phen)(Cl)$], [$Ni(L_1)(Bipy)(Cl)$] (where Phen = 1,10-phenanthroline; Bipy = 2,2'-bipyridyl, L1 ==**(2-carboxyphenyl)-pyridine-2-ylethyleneamine)** monobasic tridentate Schiff base have been synthesized by **2-Acetyl pyridine,2-Amino Benzoic Acid**. All of the new complexes have been characterized on the basis of analytical and spectral data.. The molar conductance data reveal that Cu(II) and Ni(II) complexes are ***non-electrolytes***. IR spectra show that L is coordinated to the metal ions in a ***tridentate manner*** with ONN donor sites of the carboxylate O, azomethine N and pyidine N. From the magnetic spectra, it is found that the geometrical structure of these complexes are **Octahedral.** The thermal behavior of these chelates shows that the hydrated complexes losses water molecules of hydration in the first step followed immediately by decomposition of the anions and ligand molecules in the subsequent steps. The synthesized ligands, in comparison to their metal complexes also were screened for their antifungal activity, antibacterial activity against bacterial species, *Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus pyogones* and Fungi (Candida). The activity data show that the metal complexes to be more potent/antibacterial than the parent Schiff base ligand against one or more bacterial species. Comlexes are showing ***fluorescence*** with high quantum yield.

PP 135

ANTIDIABETIC AND ANTIDYSLIPIDEMIC ACTIVITY OF MOMORDICA CHARANTIA (KARELA) FRUITS

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Diabetes Mellitus is a metabolic disorder of carbohydrate metabolism with several complications such as hyperglycemia, insulin resistance, impaired glucose tolerance, decreased hepatic glycolysis, increased gluconeogenesis and so forth. It is primarily due to impaired insulin production or action or both [1]. Various approaches to the treatment of diabetes include insulin supplementation, oral hypoglycemic agents such as sulphonylurea, metformin and thiazolidinediones and DPP-IV inhibitors [2]. Looking at the adverse side effects of these drugs in long term use herbal medicines are more preferred either solely or in combination with these agents. In the present study the aqueous extract of *Momordica charantia* (Karela) fruits were evaluated for antihyperglycemic and antidyslipidemic activity in normoglycemic rats, streptozotocin (STZ) induced diabetic rats with and without sucrose challenge, and high fructose diet (HFD) fed Sprague-Dawley rats. The extract showed significant improvement (13.9%**) on oral glucose tolerance of sucrose loaded normoglycemic rats. Significant lowering of blood glucose i.e.14.7%* and 16.3%** were also observed in STZ-induced diabetic with and without sucrose challenge, respectively. The aqueous extract also showed significant antidyslipidemic activity in HFD fed SD-rats by declining serum triglycerides level by 5.87%, 8.52%, 18.6%, 24.9% and significant decline in serum cholesterol level by 33.46%**, 19.69%*, 24.55%*, 35.04%** on 7^{th} , 14^{th}, 21^{st} and 28^{th} day post treatment. respectively. However serum HDL level was found increased by 31.8% on 28^{th} day. The hepatic and renal function parameters of STZ-induced diabetic rats were also found improved on 28^{th} day post treatment of aqueous extract of M.charantia fruits. The decrease in serum urea, uric acid, creatinine, GOT and GPT levels were calculated around 25.08%*, 21.79%*, 19.87%, 20.52%*, and 16.33% respectively. These studies warrants to look for the antidiabetic ingredients in the aqueous extract of M.charantia fruits for design of new class of antidiabetic compounds of natural origin.

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PP 136

SYNTHESIS AND CHARACTERIZATION OF AROMATIC COPOLYAMIDES CONTAINING ETHER KETONE LINKAGE AND PENDANT PHENYL GROUPS.

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Aromatic polyamides (aramides) have high temperature resistance and excellent mechanical strength but infusibility and limited solubility of aramides in organic solvents restrict applications. Efforts have been made to design the chemical structures with some pendant phenyls or flexible linkages, to obtain aramides with improved processability. Here we report synthesis and characterization of new aromatic diamine; 4, 4'-bis-(4-amino phenoxy) benzophenone (4APB); and novel polyamides therefrom. 4APB was synthesized in more than 90 % yields either by condensation of 4, 4-dihydroxybenzophenone with 4-chloronitrobenzene and subsequent reduction of intermediate dinitro-ether-ketone; 4, 4'-bis (4"nitro phenoxy) benzophenone (4NPB); with hydrazine monohydrate or by reaction of 4-aminophenol with activated dihalides; 4, 4'-difluorobenzophenone; in a polar aprotic solvent in presence of potassium carbonate. Compounds 4APB and 4NPB were characterized by FT-IR, ^{1}H, and ^{13}C NMR, and elemental analysis.

Low temperature solution polycondensation of 4APB in combination with phenylated diamine; 2, 5'-bis (4-amino phenyl) 3, 4 diphenyl thiophene (TPTPDA); in different mol %; and aromatic diacid chlorides IPC in DMAc gave the copolyamides containing ether-ether-ketone linkages in the main chain having pendant phenyl groups.

These co-polyamides had moderate to high molecular weights, with inherent viscosities in the range of 0.25 – 0.74 dL/g in NMP. The polymers were characterized by FT-IR, inherent viscosity, solubility tests, DSC, TGA and XRD. These polymers were semicrystalline as evidenced by XRD diffractograms. Polymers dissolved in polar solvents such as DMAc, NMP. Polymers showed the glass transition temperatures, 241-319 ^{0}C. Polymers were stable upto 318 ^{0}C when investigated by TGA. These new polymers are expected to find applications as gas separation membranes and engineering materials in aerospace and nuclear industries in the form of high performance films, coatings etc.

PP 137

SYNTHESIS AND EVALUATION OF SOME NOVEL BENZOTHIAZOLO SUBSTITUTED TRIAZOLES.

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Benzothiazoles and triazoles are found to possess various activities such as antimicrobial (Udapaudi et al.)[1], antitumor, antiviral and anthelmintic. In order to obtain new potent therapeutic agents we have synthesized various compounds JMS-1 to JMS-10 by conventional and microwave assisted synthesis method. In the present work 7-Chloro-6-fluoro-benzothiazol-2-yl-amine was synthesized from 3-Chloro-4-fluoro phenylamine (Patel et al.)[2]. Then we synthesized the different 1-(5-substituted-1*H*-1, 2, 4-triazol-1-yl) ethanone, from the different substituted acids which were reacted with the hydrazine hydrate, acetyl chloride and formamide. Attempts were made to synthesize various derivatives from 7-chloro-6-fluoro-benzothiazole and 1-(5-substituted-1*H*-1, 2, 4-triazol-1-yl) ethanone by creating a mannich base with the help of formaldehyde in ethanol (Bele et al.)[3]. All the titled compounds were recrystallized and characterized by spectral analysis. The melting points of all titled compounds were taken in open capillary tube and are uncorrected. Antimicrobial study shows that synthesized compounds have moderate activity against all tested microbial strains. JMS-4 and JMS-8 derivatives have shown better degree of anti-tubercular activity in all concentrations.

Keywords: Benzothiazole, 1,2,4-Triazol, Mannich base, Antimicrobial activity.

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PP 138

SYNTHESIS AND CHARACTERIZATION OF NOVEL POLYAMIDES FROM N-(3-AMINOPHENYL)-2-(4-AMINOPHENYL) ACETAMIDE

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A novel aromatic diamine containing methylene moiety, amide linkage, was synthesized from its corresponding dinitro compound and characterized by IR, ^{1}H, ^{13}C NMR and Mass Spectrometry. A series of new aromatic polyamides was prepared by low temperature solution polymerization from N-(3-aminophenyl)-2-(4-aminophenyl) acetamide and isophthaloyl chloride and / or terephthaloyl chloride in different mole proportions. These polyamides were characterized by spectroscopic technique, viscosity measurement, solubility, thermal stability and XRD. Polymers had moderate molecular weights as evidence by the inherent viscosities in the range 0.20 – 0.58 dL/g and the polymers readily dissolved in DMAc, DMSO, NMP, m-cresol and conc.H_2SO_4. Wide angle X – ray diffraction (WXRD) results showed that introduction of methylene groups into polymer chains lead to decrease in crystallinity. Polymers did not show any weight loss below 248 ^{0}C and retained 29 to 44 % weight at 850^{0}C (Char yield) when investigated by TGA under nitrogen atmosphere demonstrating good thermal stability. The structure-property relationships for the polyamides were analysed, as these polyamides are of interest as materials for electronics, microelectronics and membrane separation technique.

PP 139

THIOCYANATION OF AROMATIC COMPOUNDS BY USING IONIC LIQUID

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An efficient, rapid thiocyanation of Aromatic compounds using ammonium thiocyanate has been developed by using ionic liquid under mild condition. The corresponding aryl thiocyanates are produced in excellent yields.

In recent years, ionic liquids have received great attention in chemistry as they have been catalytic species and alternative solvents to replace the traditional solvents. These versatile properties of ionic liquids prompt chemist to carry out numerous organic reaction in the ionic liquid [1].

Aryl thiocyanates are important synthetic precursors for the preparation of sulfur-containing organic compounds. The thiocyanato group occurs as an important functionality in certain anticancer natural products, [2] also these are intermediates for a preferred synthetic route to several types of thiazoles, [3] this functional group can be used as a masked mercapto group. Aryl thiocyanates have found a wide variety of applications as insecticides, [4] biocidal, [5] antiasthmatics, [6] vulcanization accelerators, [7] and starting materials for the preparation of heterocycles. Here we report a novel, rapid and eco-friendly method for the synthesis aryl thiocyanates, using ionic liquid.

Scheme:

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PP 140

RESOLUTION OF AMINOETHYL-4-HYDROXYL METHYL QUINOLONE USING DISTERIOMERIC SALT FORMATION

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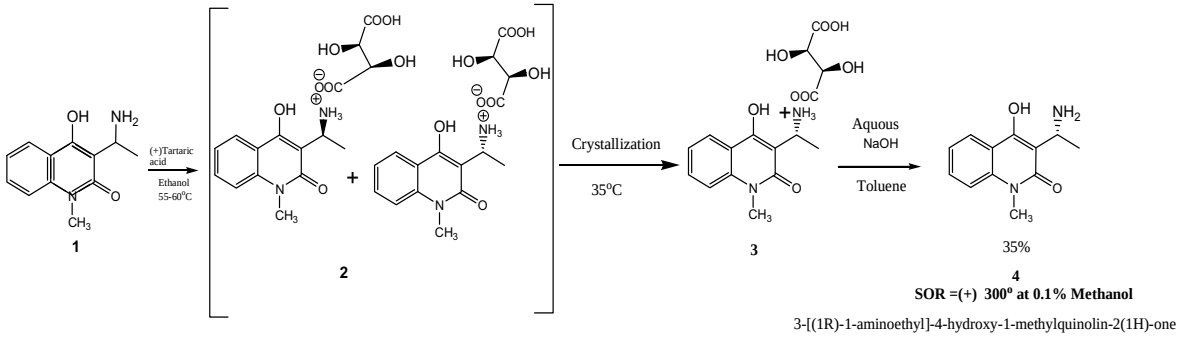
Described is an efficient and economic process for obtaining chiraly pure aminoethyl-4-hydroxyl methyl quinolone using disteriomeric salt formation. The reaction of 4-hydroxy-3-acetyl methyl quinolone and hydroxyl amine hydrochloride in presence of triethyl amine gave oxime, which on catalyticalreduction with Raney nickel in methanol, aq. ammonia and yield racemicamine of quinolone. This racemic amine was then reacted with chiral tartaric acid in ethanol via disteriomeric salt formation gavschiraly pure 4-hydroxy-3-acetyl methyl quinolone. The structureof both enantiomericcompoundswereconfirmed by specific optical rotation and chiral purity using chiral column chromatography.



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PP 141

FIRST TOTAL SYNTHESIS OF PRASINIC ACID

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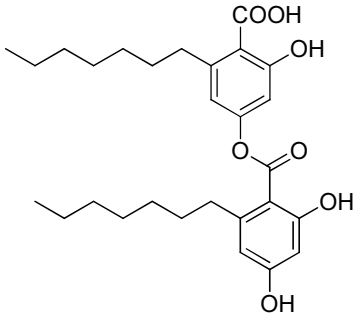
The prasinic acid (1) and two unique diphenyl ethers methoxymicareic acid and micareic acid were first isolated[1] in 1984 by Elix et.al. from Lichen Micarea prasina Fr. While, two other compounds KS-501 and KS-502, were isolated from the culture broth of fungus Sporothrix sp. These substances inhibit the activation properties of calmodulin[2,3] on the calmodulin-dependent enzymes. It has been shown that drugs that inhibit calmodulin sensitive processes are also potent inhibitors of the growth and viability of tumor cells. On this basis we assumed that prasinic acid could serve as a potential anticancer drug candidate. *S*ynthesis of prasinic acid has not been reported in literature. We wish to preset the total synthesis of prasinic acid for the first time. The ten-step procedure involves readily available, affordable starting materials and also with good yield. The crucial steps of the synthesis included the formation of two different aromatic units and their coupling reaction.



Prasinic Acid (1)

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PP 142

MECHANISM OF ELECTRICAL CONDUCTION IN SPRAYED CUINSE$_2$ THIN FILMS

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$CuInSe_2$ is the top most promising material for solar cell applications because of its high absorption coefficient, suitable band gap and good thermal, environmental and electrical stability. $Cu_{1-x}In_xSe_2$ thin films ($0 \leq x \leq 1$) with bit different approach have been selected for the studies and were prepared from $CuCl_2$, SeO_2 and $InCl_3$ as the precursors. The deposition temperature (400 ^{0}C), spray rate (5ml /min.), air pressure (1.2Kg/m^2) and nozzle to substrate surface distance (30cm) were selected as optimized. For these films, to understand the conduction mechanism, the electrical conductivity and thermoelectric power were measured in the 300 K - 500 K temperature range. The films are semiconducting in nature and show presence of defects and two types of conduction mechanisms; a variable range hopping in low temperature region whereas a grain boundary limited scattering in high temperature zone. Further, conductivity is found to be increased continuously with x up to 0.4 and then decreased for higher x- values. A highest electrical conductivity ($1.1x10^{-4}\Omega$-cm) has been observed at x=0.4. The activation energies of an electrical conduction in both temperature regions were calculated from this data. The thermopower measurements showed n (upto x=0.4) and p (x>0.4) conductions. The carrier concentration and carrier mobility were determined for all the films and their temperature dependence have been studied. The intercrystalline barrier heights were then calculated for these samples. It is found that barrier height follows the same trend of variation as that of the electrical conductivity. The results have been adequately explained.

PP 143

MICROWAVE ASSISTED SYNTHESIS OF FLOURO CHLORO BENZIMIDAZOLO SUBSTITUTED THIAZOLIDINONE DERIVATIVES FOR ANTIMICROBIAL ACTIVITIES

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Some flouro-chloro benzimidazolo substituted thiazolidinone derivatives are known to exhibit diverse bioactivities such as antimicrobial Jubie et al. [1], antifungal Ayhan et al. [2], antitubercular, anticancer, antitumour Ludmyla et al. [3], antidepression and antiviral. In view of the above moiety and in continuation of search we have prepared flouro-chloro benzimidazolo-thiazolidinone derivatives. Flouro-chloro benzimidazolo substituted thiazolidinone derivatives synthesized using microwave irradiations by reacting 3-chloro, 4-flouro ortho phenylenediamine with para-amino benzoic acid and the aspartic acid respectively followed by different aromatic aldehyde and thioglycolic acid in presence of aluminium chloride Funiss et al. [4]. The compound shows absorption bands ranging from 3433- 3320 cm^{-1} for N-H, 3149-3034 cm^{-1} for C-H aromatic stretching and 1521-1342 cm^{-1} for NO_2 functional group. In ^{1}HNMR the presence of methylene proton and methyl protons between δ 2.49 ppm and δ 3.31 ppm respectively was observed respectively. For aromatic protons multiplets were observed between δ 6.8-7.25 ppm and N-H δ 6.8ppm. A series of 12 derivatives were prepared and 10 were tested for antimicrobial activity on Gram (+ve) and Gram (-ve) bacteria. Derivatives were confirmed by TLC, Melting point, IR, NMR and Mass spectrometry. In antimicrobial activity SP103, SP203, SP206, SP207 have shown better activity against Gram negative bacteria *E coli*, and SP201 and SP207 have shown good activity against Gram positive bacteria *S. aureus*.

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PP 144

3D QSAR ANALYSIS ON TRIAZEPANE DERIVATIVES AS DPP-IV INHIBITORS

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Three dimensional quantitative structure activity relationship (3D QSAR) analysis using k nearest neighbor molecular field analysis (kNN MFA) method was performed on a series of Triazepane derivatives, Woul et al. [1] as dipeptidyl peptidase IV (DPP IV) inhibitors using molecular design suite. VLifeMDS 3.0 [2]. This study was performed with 22 compounds (data set) using sphere exclusion (SE) algorithm method for the division of the data set into training and test set. Shen et al. [3]. KNN-MFA methodology with stepwise (SW), simulated annealing (SA) and genetic algorithm (GA) was used for building the QSAR models. The predictive models were generated with SW-kNN MFA. The most significant model is having internal predictivity 72.62% (q2 = 0.7262) and external predictivity 47.06 % (pred_r2 = 0.4706).

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PP 145

EFFECT OF Sb^{3+} DOPING ON TRANSPORT PROPERTIES OF $Cd_{1-X}Hg_XS$ TERNARY FILMS

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Different semiconductor materials differ in their properties. By alloying multiple compounds, some semiconductor materials are tunable. The result is ternary, quaternary, or even quinary compositions. Quaternary and higher compositions allow adjusting simultaneously the band gap and the lattice constants, allowing increasing radiant efficiency at wider range of wavelengths. Antimony (III) doped (0.01 mol.% to 1 mol.%) $Cd_{0.92}Hg_{0.08}S$ thin films were therefore grown onto the spectroscopic glasses at the deposition conditions that are already optimized. The salts solutions of Cd, Hg and S were used for the deposition. The source of Sb^{3+} was AR grade $SbCl_3$ (99.99 %) and the calculated amount Sb^{3+} was added directly in to the reaction bath. The electrical conductivity and thermo power measurements of all these Sb^{3+} doped films were measured in the 300 K – 500 K temperature range. The temperature dependence of electrical conductivity showed an usual Arrhenius behaviour. The dependence of an electrical conductivity on antimony doping concentration showed a significant enhancement in conductivity with increasing Sb^{3+} concentration upto 0.1 mol % and further increase in doping concentration decreased the electrical conductivity. The thermoelectric power measurements showed n – type conduction. The carrier concentration (n) and mobility (μ) were then determined from the above data. Both n and μ increased with Sb^{3+} doping concentration upto 0.1 mol % and decreased thereafter. The intergrain barrier potential (Φ_B) decreased with Sb^{3+} doping concentration, attained a minimum value at 0.1 mol. % and afterwards, it increased with further increase in Sb^{3+}doping concentration in the film.

PP 146

SOME INVESTIGATIONS ON $Cd_{1-x}Co_xS$ DILUTED MAGNETIC SEMICONDUCTORS

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The recent interest in all things 'DMS' has provided a boost for liquid phase chemical bath deposition. DMS's bridge the Physics of semiconductors and magnetics since they show typical semiconductor behaviour and also reveal pronounced magnetic effects. These materials have some unique properties that enhance their potential for use in a wide range of optoelectronic devices. Here we intend to deposit CdS and $Cd_{1-x}Co_xS$ ($0 \leq x \leq 0.5$) thin films and report their electrical transport. The deposition was carried out from a complex liquid phase formed by equimolar volumes of cadmium sulphate, triethanolamine, thiourea and cobalt sulphate; all AR grade. The film composition was decided by appropriate volume of cobalt sulphate. The preparative parameters used were as-optimized earlier. The deposited samples were thin, uniform, tightly adherent and diffusely reflecting with colour changing from orange red to dark chocolate as x was varied from 0 to 0.5. The terminal layer thickness is increased initially upto 0.1 and then decreased at higher x values. The dc electrical conductivity and thermoelectric power were therefore measured in the 300 K -550 K temperature range and their temperature dependences have been studied to determine the various materials transport characteristics (activation energies, location of donor levels, intercrystalline barrier potentials, conduction mechanisms, carrier concentration and mobilities, etc). The composition dependence of an electrical conductivity revealed decrease in conductivity upto x=0.1 and remained more or less constant beyond. Thermoelectric power measurements showed an increase in TEP with temperature showing n-type conduction. For all the samples, the remarkable result is that carrier concentration and mobility increased significantly with temperature , whereas a considerable decrease in them has been observed for increasing film composition, x.

PP 147

APPARENT MOLAR VOLUME AND VISCOSITY B-COEFFICIENT OF POTASH ALUM IN WATER AND WATER + N, N-DMF MIXED SOLVENT AT DIFFERENT TEMPERATURES

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Measurements of densities and viscosities of potash alum in water and water + (0 %, 5%, 10 %, 15 % and 20%) N,N-dimethylforamide have been made as function of molality at T = (298.15, 303.15, 308.15, and 313.15) K and at atmospheric pressure. Density data have been used to calculate the partial molar volumes of potash alum. Viscosity data have been analysed by using Jones-Dole.equation and B coefficients have been calculated. Partial molar volumes and B coefficients have been used to draw the conclusions regarding structure making or breaking behavior of potash alum.

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PP 148

SYNTHESIS AND CHARACTERISATION OF NOVEL COPPER COMPLEXES OF SULPHONYL UREA DERIVATIVES AS AN EFFECTIVE HYPOGLYCEMIC AGENT

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The present communication reports the synthesis and characterizations of novel copper complexes of sulphonyl urea. The complexes were found to be novel and can be prepared by the reaction of sulphonyl urea derivatives with copper salt. The spectral and elemental analysis confirmed the structure of complexes. The synthesized compounds were screened in vivo studies for their hypoglycemic activity. It has been found that the complexes of copper show the remarkable activity than parent sulphonyl urea derivatives.

PP 149

SYNTHESIS AND CYTOTOXIC ACTIVITY OF SOME RUTHENIUM (II) COMPLEXES

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Cancer is a disease characterized by uncontrolled proliferation of cells. Anand et al. [1]. Ruthenium exists in both Ru(II) and Ru(III). Derivatives of bipyridine and terpyridine are numerous Cotton et al. [2]. Ruthenium possess a strong complex forming ability with numerous ligands. Gopal et al. [3]. Thirteen ruthenium complexes of the type $Ru[(L)_2(L_1)]^{2+}$ were prepared by reacting $Ru(L)_2Cl_2$ (where L= 2,2'-bipyridine (byp)/1, 10-phenanthroline (phen) Dimethylsulfoxide (DMSO) with ligands L_1 = BT, HBT, FCl- BT (RB), FCl-HBT, IINH, NO_2-MPC, OCH_3-MPC, DM-MPC, Cl-MPC (where BT= benzothiazole, HBT= hydrazinobenzothiazole, fluoro-chlorobenzothiazole, fluro-chloro-2-hydrazino benzothiazole, IINH= N-2-oxo-1,2-dihydro-3H-indol-3-ylidene]pyridine – 4- carbohydrazide, NO2- MPC = N(4-nitrophenyl)-methylidine-pyridine-4-carbohydrazide, OCH_3- MPC= N(4-methoxyphenyl)-methylidene-pyridine-4-carbohydrazide, DM-MPC = (N (4-dimethylaminophenyl)methylidene pyridine-4-carbohyrazide, Cl- MPC = N(4-chlorophenyl)methylidene- pyridine- 4- carbohydrazide. Structures of all these complexes established by IR, ^{1}H-NMR, &mass spectroscopy. The ruthenium (II) complexes were evaluated for their preliminary cytotoxic activity against murine leukemia cells (L1210), and human T-Lymphocytes cells (CEM) and human cervix carcinomas cells (HeLa) Karki et al. [4]. Amongst all, TKA-9 exhibited cytotoxicity at 5.5μM in comparison with standard melphalan (2.1 to 3.2 μM). Further study is under progress to understand mode of action in our laboratory.

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PP 150

SYNTHESIS AND ANTICANCER ACTIVITY OF 2,5,6 TRI-SUBSTITUTED IMIDAZO[2,1-B]-1,3,4-THIADIAZOLE DERIVATIVES.

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Mutation leading to change in nucleotide sequence of genetic material is one of the major causes for cancer. Treating cancer at molecular level is the soul of present research work. Based on the promising result reported by Karki et al.[1] for imidazo[2,1-b]-1,3,4-thiadiazoles as anticancer, a series of 2,5,6-trisubstituted imidazo[2,1-b]-1,3,4-thiadiazole derivatives have been synthesized by reacting 2-amino-1,3,4-thiadiazole with different α-bromoacetophenones. Further bromination, thiocynation, and formyaltion were carried out at 5th position of parent molecule to correlate structure with biological activity. Structures of the synthesized derivatives were established by IR, ^{1}H NMR, and mass spectra. All the compounds were tested at the National Cancer Institute on a panel of 60 human tumor cell lines.[2]. The compound with pre-determined threshold inhibition criteria in a minimum number of cell lines, progress to the full 5-concentration assay. 2-benzyl-6-(4'-chlorophenyl)-imidazo[2,1-b][1,3,4]thiadiazole showed potent antitumor activity and was selected by the Biological Evaluation Committee for an *in-vivo* test.

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PP 151

COMPARATIVE STUDY OF CALCIUM BASED AYURVEDIC DRUG KAPARDIKA BHASMA AND PURE CALCIUM CARBONATE

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Kapardika Bhasma is one of the important calcium based ayurvedic drug of marine origin. It is prepared from naturally occurring *Karardika (Varatika)* by following traditional process of *Bhasmikarana*. This traditional ayurvedic process involves three major steps (i) Selection of an appropriate sample of *Kapardika* according to directions given in Ayurvedic literature and its purification called as *Shuddhi*. (ii) Conversion of this purified material into finely powdered state. (iii) Transformation of this powder into final *Bhasma* state by following ayurvedic process of *Bhasmikaran*a.

Excellent medicinal properties are ascribed to a genuine *Kapardika Bhasma* which include (i) antacid behavior (ii) Skin Infection especially Skin burning. (iii) chronic loss of apatite and (iv) Stomach ache induced after the meals (called as *parinamashula*).

From chemical point of view, *Kapardika Bhasma* is predominantly composed of calcium carbonate (95%) as its major constituent along with magnesium and Silica as the minor constituents (2-3%) and a number of trace constituents. Apart from these it is expected that organic component, which is invariably present in the original sample of *Kapardika*, should be present whose presence and important role is totally neglected up-till now.

All these properties are quite different than pure calcium carbonate and cannot be attributable to other minor or trace constituents alone. Therefore, a comparative study of *Kapardika Bhasma* and pure calcium carbonate is carried out with a specific objective to search the factors which are behind the differential behavior and the characteristic medicinal properties of *Kapardika* Bhasma.

PP 152

ALIPHATIC-AROMATIC CARDO AND PHENYLATED POLYAMIDES FROM 2, 3 –BIS - [(4”-AMINO PHENOXY)-4’ PHENYLENE] QUINOXALINE.

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A new quinoxaline moiety containing aromatic diamine; 2, 3- bis-[(4”- amino phenoxy) - 4’-phenylene] quinoxaline (APQ) was synthesized starting from 4-methoxybenzaldehyde and was characterized by FT-IR, ^{1}H, ^{13}C NMR and Mass spectrometry. Four new polyamides were synthesized by polycondensation of various aliphatic diacid / aromatic diacids namely, adipic acid, sebasic acid; 1,1’ Bis[4’’-(4-carboxy methylene phenoxy phenyl)] cyclohexane and 2,5 Bis(4- carboxy methylene phenyl) - 3,4 diphenyl thiophene with APQ by Yamazaki’s phosphorylation method using triphenyl phosphite as condensing agent. The polyamides were characterized by FT-IR spectroscopy, solubility tests, inherent viscosity, X- ray diffraction technique, differential scanning colorimetry and thermogravimetric analysis. The polyamides had inherent viscosities in the range 0.35-0.49 dL/g in N, N-dimethylacetamide at 30 ± 0.1 °C. The polyamides were soluble in polar aprotic solvents such as N, N-dimethylacetamide, N, N-dimethylformamide, dimethylsulfoxide, N-methylpyrrolidone, Pyridine and m-cresol. X-Ray diffraction studies showed that polyamides were amorphous in nature. The polyamides showed glass transition temperatures in the range 146- 154 °C, according to differential scanning calorimetry. Thermogravimetric analysis exhibited initial decomposition temperatures above 324 °C; and the char yield at 900 °C was in the range 30-62 % indicating that these polyamides possessed excellent thermal stability.

PP 153

SYNTHESIS AND CHARACTERIZATION OF POLY(ESTER-URETHANE)S AND ITS USE AS A CONTROLLED DRUG RELEASE MATRIX.

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New biodegradable poly(ester – urethane)s derived from dimers of lithocholic acid were synthesized. As lithocholic acid is hydrophobic in nature and with urethane linkage attached it becomes more hydrophobic, the lithocholic acid dimer was condensed with various hydrophilic diols (such as PEG-400, PEG-600, PEG-800, 1,4-butane diol and 1,6-hexane diol) to reduce the hydrophobicity of the polymers. These polymers containing ester urethane linkage were synthesized using dibutyl tin dilaurate (DBTDL) and dibutyl tin oxide (DBTO) as urethanation and esterification catalyst. The polymers were characterized by IR and ^{1}H NMR spectroscopy and their solubility was checked in various solvents. The release of paracetamol as a model drug was studied at two different pH (1.2 and 7.4) by using the above polymers as excipients. The release studies show that due to presence of hydrophobic segments in the polymers the release of drug occurs over extended period. Therefore, these polymers can be used as matrix for sustained drug delivery.

PP 154

EXTRACTIVE PHOTOMETRIC DETERMINATION OF Zn(II) WITH BIS-[4-(N-2'-HYDROXY BENZILIDINE IMINO) DIPHENYL] ETHER

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Salicyladehyde and 4,4'-diaminodiphenyl ether(ODA) were reacted in 2:1 mole ratio to obtain an O N doner schffs base with bis-[4-(N-2'-hydroxy benzilidine imino)diphenyl] ether(SOADA).SOADA forms yellow coloured complex with Zn(II) in basic medium which can be extracted in chloroform and Zn(II) was determined spectrophotometrically at λmax 405 nm. The Sandell's sensitivity of the method was found to be 40 ng / cm^{-2} at 405 nm and molar absorptivity was found to be 1630 L mol^{-1} cm^{-1}. Beer's law validity range is found up to 200µg. Zinc(II) forms 1:2 (M:L) complex with the legend. The proposed method is rapid, reproducible and has been satisfactorily applied to the determination of trace amount of Zinc in synthetic mixture.

PP 155

SYNTHESIS, SPECTRAL ANALYSIS AND ANTIMICROBIAL ACTIVITY OF SOME NEW TRANSITION METAL COMPLEXES DERIVED FROM 2, 4-DIHYROXY ACETOPHENONES

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Cu (II), Ni (II), Co (II), Fe (III), Zn (II) and Mn (II) complexes were synthesized from Schiff bases derived from 2-amino pyridine and 2, 4-dihydroxy acetophenone. The structures of the complexes have been characterized by elemental analysis, conductometry, thermal analysis, magnetic measurements, IR, ^{1}H NMR, UV-Vis spectroscopy and a microbial study.

From the analytical and thermal data, the stoichiometry of the complexes was found to be 1:2 (metal:ligand). The molar conductance data revealed that all the metal chelates were non-electrolytes. The thermal stability of the complexes was studied by thermogravimetry and the decomposition schemes of the complexes are given. The ligands and their metal complexes were screened for antibacterial activity against various bacteria like *E coli*, *S. typhi*, *S. aureus*, *B. subtilis* at various concentrations, Similarly the same compounds were screened for the antifungal activity against different organisms like *P. chrysogenum*, *A. niger*, *F. moniliformae*, and *C. albicans.* Metal complexes showed enhanced antimicrobial activity than their corresponding ligands.

PP 156

AN EFFICIENT SYNTHESIS OF 5,7-DIPHENYL-2-THIOXO-2,3-DIHYDROPYRIDO[2,3-d]PYRIMIDIN-4(1H)-ONE DERIVATIVES IN IONIC LIQUID

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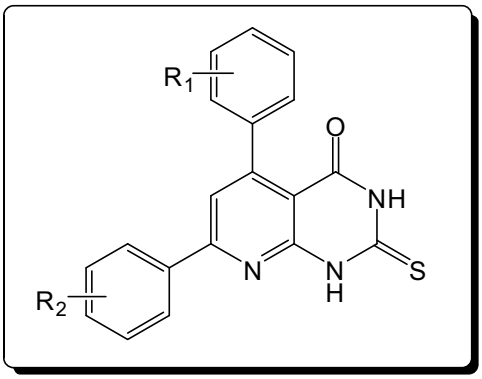
Pyrimidine and thienopyrimidine derivatives have attracted a great deal of interest owing to their medicinal activities. Pyrimidine derivatives and heterocyclic annelated pyrimidines continue to attract great interest due to the wide variety of interesting biological activities observed for these compounds, such as anticancer, antiviral, antitumor, anti-inflammatory and antimicrobial activities. In a view of great importance of pyridipyrimidinones, we report herein a simple, efficient, rapid and high yielding protocol for the synthesis of 5,7-diphenyl-2-thioxo-2,3-dihydropyrido[2,3-d]pyrimidin-4(1H)-one derivatives using ionic liquid as green and recyclable reaction medium.



PP 157

SIGNIFICANCE OF ANTIOXIDANT ENZYMES IN STRESS SIGNALING

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Plant expose to stress undergo changes in their metabolism in order to adapt to the changes in their environment. The present study was conducted to reveal the role of antioxidant enzymes like superoxide dismutase and peroxidase during acetyl salicylic acid and NaCl signaling in W. sominifera (L.) Dunal. Using enzyme activity staining on acrylamide gels. The results showed that during acetyl salicylic acid signaling, SOD activity increased in 2nd & 4th hrs and decreased till 6th hrs and further increased up to 10th hrs. Similarly in peroxidase, a low enzyme activity was observed in 0 and 6th hour while in 2nd, 4th, 8th and 10th hour the expressions of three isozymes of peroxidases were observed. Activity by 6th hour may result in increased accumulation of H2O2 resulting in oxidative burst. The decrease in SOD activity may be due to the feedback inhibition mechanism of the enzyme. During NaCl stress only SOD activity was calized since POD activity was negligible. In different NaCl concentration from 1000 to 6000 ppm, the SOD activity was maximum increase during 5000 ppm treatment revealed by the presence of three bands. During time dependent NaCl treatment, the SOD activity increased during 2nd to 8th hour of treatment revealed by the presence of two bands. The result in the present study highlight a probable occurrence of oxidative burst in Withania sominifera (L.) during 4th and 6th hours of stress signaling. Sometimes high amount of H2O2 accumulated and generating PCR/HR signals against plant pathogens to protect plant.
Keywords: Withania sominifera, Antioxidant, Superoxide Dismutase (SOD), Peroxidase (POD), Acetyl salicylic acid, diaminobenzedene (DAB), Tetramethylene benzedene (TMB)

PP 158

ANTIHYPERGLYCAEMIC ACTIVITY IN NYMPHAEA RUBRA AND JATROPHA GOSSYPIFOLI*A*

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As a prelude to discover antihyperglycaemic activity in terrestrial plants, two new antihyperglycaemic plants were identified as Nymphaea rubra and Jatropha gossypifolia. The ethanolic, aqueous and aqueous extracts of the flowers of N. rubra and aqueous and alcoholic/aqueous extracts of stem of J.gossypifolia showed improvement on oral glucose tolerance in both normoglycaemic as well as streptozotocin-induced diabetic rats. Significant blood glucose lowering activity was also observed with each of the extracts on STZ-induced diabetic rats. In order to enrich the antihyperglycaemic activity the ethanolic, aqueous and alcoholic/aqueous extracts of both N.rubra flowers and J. gossypifolia stem were further fractionated with hexane, chloroform, butanol and water. The chloroform fraction of alcoholic extract of J. gossypifolia showed significant improvement on oral glucose tolerance in both normal and streptozotocin-induced diabetic rats whereas both chloroform and butanol fractions of the aqueous extract of J.gossypifolia showed significant improvement on oral glucose tolerance in both normoglycaemic as well as streptozotocin-induced diabetic rats. Though the alcoholic/aqueous extract of stem of J.gossypifolia found ineffective, showed significant improvement on oral glucose tolerance in both normoglycaemic and streptozotocin-induced diabetic rats. These fractions also showed demonstrable blood glucose lowering activity on streptozotocin-induced diabetic rats. The chloroform and aqueous fraction of the alcoholic extract, hexane aqueous extract of the aqueous extract and aqueous fraction of alcoholic/aqueous extract of N. rubra flowers showed significant improvement on oral glucose tolerance in both normoglycaemic and streptozotocin-induced diabetic. The chloroform fraction of the alcoholic extract, hexane and aqueous fractions of aqueous extract and aqueous fraction of aqueous extract of N.rubra flowers showed improvement on oral glucose tolerance in both normoglycaemic and streptozotocin-induced diabetic rats. A comparison of blood glucose lowering of fractions of the extracts of N.rubra flowers and J.gossypifolia stem revealed almost equal activity in chloroform fraction of alcoholic extract and aqueous fraction of alcoholic extract of J.gossypifolia flowers and hexane and aqueous fraction of aqueous extract of N.rubra flowers and butanol fraction of the aqueous extract of stem of J.gossypifolia on streptozotocin-induced diabetic rats Experiments are in progress to explore the mechanism (s) of antihyperglycaemic action of these fractions of N.rubra flowers and J.gossypifolia stem.

PP 159

HETEROPOLYACID CATALYZED OXIDATION OF ALCOHOLS, CHLORIDES TO CORRESPONDING ACIDS USING OXONE IN AQUEOUS ACETONITRILE

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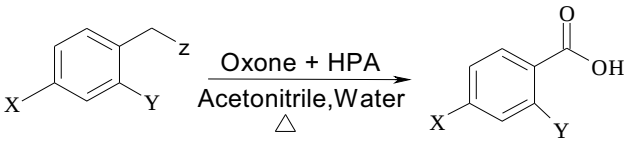
Oxidation of alcohols and chlorides is one of the important pathways for the generation of carbonyl compounds that find wide applications in synthetic organic chemistry [1]. Oxone, a stable ternary composite of K_2SO_4, $KHSO_4$ and $KHSO_5$ in 2: 1: 1 proportion and is peroxy oxidant available commercially. Although Oxone has been used earlier in the oxidation of secondary alcohols, sulfides, etc.[2,3,4,5] its use in the oxidation of primary aromatic alcohols and benzyl chlorides has not yet been explored. In continuation with our work on solid acid catalyst [6] herein we report hetropolyacid catalyzed, efficient protocol for oxidation of benzylic alcohols as well as chlorides to corresponding acids in aqueous acetonitrile medium. Simple reaction procedure, high yields in very short time are the major merits of the developed protocol.



X, Y = Cl, Br, F, NO_2, CH_3, H

Z=Halogen / OH

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PP 160

STRUCTURAL AND OPTO-ELECTRICAL PROPERTIES OF NANOCRYSTALLINE INDIUM SELENIDE THIN FILM

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Nanocrstalline In_2Se_3 semiconducting thin films were prepared by using relatively simple chemical bath deposition method at room temperature by the reaction between indium chloride, tartaric acid, hydrazine hydrate and sodium selenosulphate in an aqueous alkaline medium. Various preparative conditions of thin film deposition are outlined. The as grown films were found to be transparent, uniform, well adherent and red in color. The films were characterized using X-ray diffraction (XRD), scanning electron microscopy, atomic absorption spectroscopy and energy dispersive atomic X-ray diffraction (EDAX). The XRD analysis of the film showed the presence of polycrystalline nature with hexagonal crystal structure. SEM study reveals that the grains are homogenous, without cracks or pinholes and well covers the glass substrate. The optical absorption and electrical conductivity was measured.. Room temperature deposition results in nanocrstalline In_2Se_3 thin film with the Hexagonal crystal structure and crystallite size of about 20.7 nm. The direct optical band gap value for the films was found to be of the order of 2.35 eV at room temperature and have specific electrical conductivity of the order of 10^{-2} $(\Omega\ cm)^{-1}$ showing n-type conduction mechanism. The utility of the adapted technique is discussed from the view-point of applications considering the optoelectric and structural data.

PP 161

SYNTHESIS AND CHARACTERIZATION OF THE SYSTEM $ZN_{1-X}CU_XFECRO_4$ PREPARED VIA SOL-GEL METHOD

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Oxides having spinel structure are some of the most studied compounds in materials science due to their wide range of applications. In this, the system $Zn_{1-x}Cu_xFeCrO_4$ was prepared by sol-gel auto-combustion method. The formation of spinel phase was identified using X-ray diffraction technique. All the compounds exhibited cubic spinel symmetry and lattice constant shows the decreasing trend with substitution of nickel. The morphology and size of the particles was found by scanning electron microscope while elemental compositions by elemental dispersive X-ray spectroscopy. Electrical and magnetic properties of the system were investigated by using the compounds in the form of pellets.

PP 162

EFFECTS OF METAL-BASED NANOPARTICLES ON MICROBIAL DIVERSITY OF SOIL

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Nature is replete with examples of a wide range of organic and inorganic nanoparticles that may play pivotal roles in many natural phenomena. However, human scientific endeavours, the ever-increasing needs of the society and creation of material wealth pose severe threats to the environment. The focus of the present studies was to determine effects of metal-based nanoparticles on biodiversity, using the soil microcosm as a model ecosystem. Such studies are important in order to determine fate of nanoparticles in the environment after their use.

Different types of nanoparticles were synthesized in our laboratory for various prospective applications, viz. reduced FeSNPs for decolorization of azo and non-azo dyes, paramagnetic NPs for environmental and biomedical applications, ferrite NPs for gas sensing and AgNPs for therapeutics. The nanoparticles were added to fertile soil samples at varying doses and the soil samples were kept under humid conditions with proper ventilation. Soil samples removed intermittently were spread on different agar media and incubated at 37ºC. The different types of bacterial/fungal colonies were identified and counted using routine morphological and biochemical analysis and individual numbers of the colonies were recorded. Soil samples with addition of plain distilled water were also included in the experiment as controls. Based on the results, the microbial species diversity was estimated using well established statistical models. The AgNPs were found to reduce the microbial diversity, while ferrite and magnetic nanoparticles were safer to the microbial communities. Reduced iron-based nanoparticles were found to exert similar effects. The results definitely point to the importance of carrying out such analyses for a variety of material being manufactured commercially.

PP 163

FORMULATION DEVELOPMENT OF MEDICATED LOLLYPOPS FOR CHILDREN

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Poor fixation of dentures in children often causes dental disorders. Ketoconazole was formulated as a lollypop to provide slow release medicament for the treatment of oral thrush in pediatric patients. There are dosage forms like syrups, tablets in the market but still there is a need for new dosage forms which acts effectively and locally. So the present investigation aims to design, prepare and evaluate Ketoconazole lollypop for increased bioavailability, reduction in gastric irritation bypassing first pass metabolism. The lollypops were prepared with and without added polymers by heating and congealing method in a candy based industry on request using liquid glucose as base. All the formulations prepared were subjected to various physico-chemical parameters like hardness, content uniformity, friability, weight variation etc. The prepared formulations have a hardness of around 12 Kg/cm², as per ICH guidelines. Stability study of selected formulations was also carried out at 37ºC for a period of six months. Selected formulations were tested for drug excipient interactions subjecting to IR Spectral analysis. In-vitro drug dissolution studies showed 86.12% for F_1 and 77.96% for F_2 release of drug in 30 minutes, 95.01% in 7 minutes from F_0 formulation. The lollypops will provide an attractive alternative formulation in the treatment of oral thrush in pediatric patients.

PP 164

Breeding Sites of Mosquitoes with reference to larval diversity at Barshi City

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We can successfully control the mosquitoes at their larval stage. For proper utilization of Larvicide, we must know: which mosquito species are locally present, where the breeding sites of these mosquito species are located. Survey on breeding sites of larvae was conducted in 5 selected sites at Barshi city. Sampling was carried out by dipping using pipette or dipper depending on breeding site. All breeding sources of mosquito larvae were grouped into 11 types: container, domestic water basin, concrete tanks, plant pots, broken pipes, tyres, seepages at homes and lake, pond, well and small water bodies at respective area. In one area, 10 homes were surveyed considering all possible breeding sites. This study indicated that the people who have underground covered concrete tank have less infestation of larvae. Whereas the people who have plastic and soil-container, domestic water basin in homes and small water bodies (Stream) in areas has large infestation of mosquito larvae. The collected mosquito larvae from indoor breeding sites belong to species of *Aedes*, *Anopheles* and *Culex* whereas species of *Aedes* from a Stream throughout five sampling sites.

PP 165

SYNTHESIS AND ANXIOLYTIC ACTIVITY OF SOME ARYLOXYPROPANOLAMINE DERIVATIVES

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In an attempt to design novel anxiolytic agents, a series of 1-aryloxy-3-(N^4-substituted piperazinyl) propan-2-ols (aryloxypropanolamines) were synthesized. 1-aryloxy-3-(N^4-substituted piperazinyl) propan-2-ols were synthesized by reaction between various substituted phenols and epichlorhydrin to give 1-aryloxy-2,3-epoxy propane. These epoxides on condensation with substituted piperazines resulted in derivatives with promising anxiolytic activity. All synthesized compounds were characterized by spectral studies. Evaluation for anxiolytic activity was done by elevated plus maze & hole board test. Some of the substituted aryloxypropanolamines derivatives have shown good anxiolytic potential.

PP 166

SYNTHESIS OF N-CONTAINING THIAZOLIDINONES VIA SCHIFF BASE FORMATION FOR BIOLOGICAL EVALUATION

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Nitrogen containing heterocyclic compounds is indispensable structural unit for both the chemist & biochemist. Recently, Thiazolidinone derivatives have been described as compounds with pluripotent biological properties[1] . The glitazones , structurally related to those compounds **(glitazone I)** are also known for their activities against colon cancer cell lines[2] . Five member nitrogen & sulphur containing thiozolidinone ring attached with other heterocyclic system have also been found with spectrum of pharmacological activities *Viz* .antibacterial , antifungal [1] anti-inflammatory, anti HIV, etc.

Keeping the above facts in view, it was thought worthwhile to design the synthesis of thiazolidinone rings in order to find new biologically active compounds. Since our group is interested in heterocycles like thiophenes, selenophenes, thiazoles and especially in condensed heterocyclic systems; here we report the synthesis of new Thiazolidinone derivatives and their biological evaluation.

In this study we have designed and synthesized novel thiazolidinones by refluxing p-amino benzonitrile with various heterocyclic aldehydes in alcohols furnished respective Schiff' bases. These Schiff bases were cyclized by refluxing with thioglycolic acid to afford thiozolidinones**,** which can be useful for the in-vitro biological evaluation..

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PP 167

AN ATOM EFFICIENT, SOLVENT-FREE SYNTHESIS OF SOME NEW HETEROCYCLIC IMINES AND ANTIBACTERIAL ACTIVITY

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A solvent-free condensation of substituted aryl amines with indole-3-aldehyde in presence of catalytic amount of acetic acid at room temperature in combination with grinding to yield new series of heterocyclic imines (Schiff bases). The simple reaction procedure, short reaction time, no need of organic solvent and high yields make this protocol practical and economically attractive.

PP 168

SYNTHESIS OF 3-BROMOIMIDAZO[1,2-*A*]PYRIDINE DERIVATIVES VIA *INSITU* OXIDATION OF HBR BY NITRIC ACID

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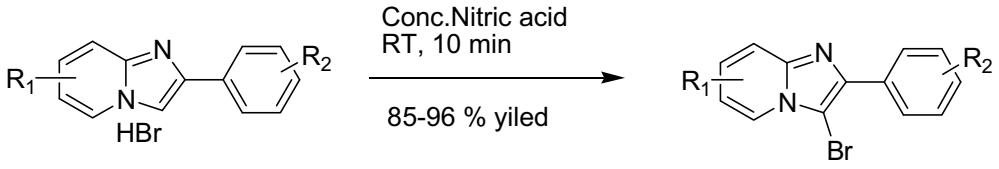
The imidazo[1,2-a]pyridine scaffold when functionalized appropriately is a starting point for preparation of a plethora of biologically active molecules. Appropriately functionalized imidazo[1,2-a]pyridine are also an attractive building block for the synthesis of tricyclic heterocycles. Herein an efficient, a novel synthesis of 3-bromoimidazo[1,2-a]pyridines is being reported with an excellent yields. The method involves insitu generation of HBr which is further utilized for bromination in presence of Nitric acid as an oxidant.



PP 169

CYANURIC CHLORIDE CATALYZED SYNTHESIS OF OCTAHYDROQUINAZOLINONE DERIVATIVES IN AQUEOUS MEDIA

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The dihydropyrimidone derivatives are found as core units in many marine alkaloids, which have been found to be potent HIVgp-120CD_4 inhibitors. In recent years, these compounds are known to exhibit a wide range of biological activities such as antiviral, anticancer, antitumer, antibacterial and anti-inflammatory, calcium channel blockers, α-1a-antagonists. Recently, the improved synthetic methodologies have been reported, most commonly Lewis acids, ionic liquids, acidic montmorrillonite KSF, MW irradiation, There are numerous methods have been developed for the synthesis of octahydroquinazolinone derivatives. There are very few reports are observed for the synthesis of octahydroquinazolinone derivatives using catalysts such as TMSCl, Nafion H, Conc. H_2SO_4 and SiO_2-H_2SO_4 , ionic liquids under ultrasound irradiation.

However, many of these reported methods have some drawbacks. Therefore, the development of efficient and versatile catalytic system for multi-component reaction is an active ongoing research area and then there is a scope for further improvement towards milder reaction conditions, variations of substituents in all compounds. We present cyanuric chloride (TCT/ 2, 4, 6-trichloro-1, 3, 5-triazine) catalyzed efficient protocol for the synthesis of octahydroquinazolinone derivatives in water with enhanced reaction rates and high yields. Cyanuric chloride is safe and highly inexpensive reagent.

PP 170

SYNTHESIS OF AMIDE DERIVATIVES OF MEFENAMIC ACID AS POTENTIAL PRODRUG

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In the past few decades, Prodrug has been extensively and successfully used as a chemical tool for modification of the physicochemical, pharmacokinetic as well as pharmacodynamics characteristics of drug molecules. Mefenamic acid is 2-(2,3-dimethylphenyl)aminobenzoic acid and it is a non-steroidal anti-inflammatory drug used to treat pain, including menstrual pain. It is typically prescribed for oral administration. This drug may infrequently cause serious (rarely fatal) bleeding from the stomach or intestines due to carboxylic acid group by direct contact mechanism. The present investigation concerns synthesis and development of amide derivatives of mefenamic acid as a potential prodrug with the aim of reduced gastric irritation. This study involves synthesis of a series of amide derivatives of mefenamic acid by first preparing mefenamic acid chloride and then reacting it with appropriate aliphatic and aromatic amines. The required mefenamic acid chloride is prepared by reacting acetyl chloride with mefenamic acid. Their structures were confirmed by spectral studies.

PP 171

PANCREATIC β-CELL PROTECTIVE AND REGENERATIVE EVALUATIONS OF GYMNEMA SYLVESTRE EXTRACT

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Gymnema sylvestre (Asclepiadaceae) is emerging as a potential treatment for the management of diabetes mellitus. The leaves are used in herbal medicine preparations. The aim of the present study was to identify the potential ability of Gymnema sylvestre to regenerate pancreatic β-cells. In the current investigation, an active extract of Gymnema sylvestre with the dose of 200 and 400 mg/kg was administered orally to steptozotocin induced diabetic rats for 40 days for the assessment of plasma glucose, insulin, glycosylated hemoglobin (HbA1c), tissue and liver glycogen, lipid parameters such as triglycerides, total cholesterol, LDL-cholesterol, and HDL-cholesterol in normal as well as steptozotocin diabetic rats. These results indicate that Gymnema sylvestre extract shows significant change in the all above said biochemical parameters when compared to control group. The histopathological study shows the significant recovery of damaged β-cells in diabetic Gymnema sylvestre treated rats, when compared to diabetic control ones. In conclusion these results indicate that Gymnema sylvestre extract, possessed hypoglycemic and hypolipidemic activity in long-term treatment and is also capable of regenerating β-cells and hence it could be used as a drug for treating diabetes mellitus. Because it has regenerating ability of β-cells, at least the people in the earliest stages of the disease could be treated to delay or prevent full-blown clinical diabetes.

PP 172

SYNTHESIS OF DIHYDROPYRIMIDINONES WITHOUT ANY SOLVENT OR CATALYST AND ITS SUBSTITUTED REACTIONS

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Multicomponent reactions (MCRs) are of increasing importance in organic and medicinal chemistry. MCR strategies offer significant advantages over conventional linear-type synthesis. In such reactions, three or more reactants come together in a single reaction vessel to form new products that contain portions of all the components. In an ideal case, the individual building blocks are commercially available or are easily synthesized and cover a broad range of structural variations.

A simple, efficient, green, and cost-effective procedure has been developed for the synthesis of dihydropyrimidinones by a solvent-free and catalyst-free Biginelli's condensation of 1,3-dicarbonyl compound, aldehyde, and urea. This approach of direct reaction in neat without solvent and catalyst shows a new direction in green synthesis. In a typical experimental procedure, a mixture of 1,3-dicarbonyl compound, aldehyde, and urea was heated at 100-120 □C without any solvent or catalyst. The reactions are completed in one hour, and the solid products was filtered and recrystallized from ethanol. It has also been observed that under identical reaction conditions (without an acid catalyst) the reaction did not progress at all in refluxing dichloromethane, dichloroethane, THF, and toluene during one hour, although refluxing for 5 h in toluene furnished 15-20% yields. This indicates the special advantage of the solventless reaction and the negative role of solvent at least in this case. A broad range of structurally diverse 1,3-dicarbonyl compounds, aldehydes, and urea are subjected under this procedure to produce the corresponding dihydropyrimidinones. The formed product was reacted with different active methylene compounds, phenols, amines and heteryl amines to give different substituted products. These newly synthesized compounds were evaluated for antibacterial activity.

PP 173

3^2 -FULL FACTORIAL DESIGN AND *IN VIVO* PHARMACODYNAMIC EVALUATION OF LIQUI-SOLID FORMULATION OF GLIPIZIDE FOR SOLUBILITY ENHANCEMENT

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Liquisolid technique is emerging technique for solubility enhancement as well as controlled release formulations along with acceptable flow properties and compressibility. The purpose of present study was to improve dissolution of Glipizide through liquisolid technique and investigate their *in vitro* and *in vivo* performance. The technique brings out conversion of liquid medications in non-volatile vehicle into powder. The mathematical model by Spireas with a 3^2-full factorial design was employed for study design using percentage of drug in liquid medication and carrier to coat ratio as two independent variables. FTIR spectroscopy and DSC study showed drug-excipient compatibility. Liquisolid preparations were characterized by precompression study for flowability and compressibility. The formulations were found to possess good flow characteristics as well as satisfactory compressibility. The DSC thermograms systems indicate the presence of dissolved drug in PEG 200. Drug release rates were found to be enhanced in case of all liquisolid formulations. The factorial equation shows that drug release is dependent on both factors. Increased carrier: coat ratio and decreased drug concentration in liquid medication demonstrated increased dissolution rates. Stability study showed that assay was not affected suggesting chemical stability in accelerated conditions. Hardness and disintegration time were found to be increased during exposure to accelerated temperature and humidity. *In vivo* pharmacodynamic study performed on wistar rats with alloxan induced diabetes shows that the liquisolid system was effective to reduce the blood glucose level. Thus, in conclusion, liquisolid formulation of glipizide is efficient to enhance dissolution with acceptable flow and compressibility.

PP 174

AN EFFICIENT GREEN SYNTHESIS, CHARACTERIZATION AND MOLECULAR MODELLING STUDIES OF FLUORO SUBSTITUTED PYRAZOLINE DERIVATIVES

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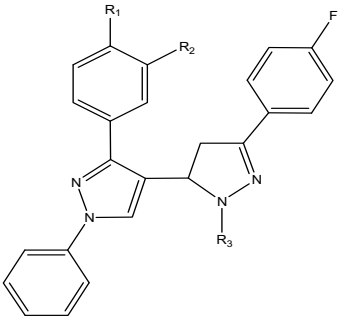
Heterocyclic compounds are known for wide range of biological activities. Now a day's much attention is being paid for the synthesis of such heterocyclic compounds containing nitrogen like pyrazoline due to its important role in medicinal chemistry. These compounds possess antimicrobial, antidepressant, anti-inflammatory1, antitumor, analgesic and antioxidant2 activities. These findings have promoted us to synthesize variety of fluorine substituted pyrazolines. Different substituted chalcones were condensed with phenyl hydrazine and hydrazine hydrate in PEG-400 (a green solvent) with few drops of acetic acid afford the pyrazoline derivatives.

It has been reported that these pyrazoline derivatives could play an important role in the treatment of hyperuricemia and have an inhibitory effect on enzyme xanthine dehydrogenase3. Hence, molecular docking using Auto Dock 4.0 has also been performed to find out the interactions between enzyme and pyrazoline derivatives and to see their inhibitory effects to cure some deadly diseases such as cancer and neurological disorders. Newly synthesized compounds were analysed by IR, 1H NMR and LCMS spectral techniques.



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PP 175

PESTICIDE USE AND HEALTH RISK ASSESSMENT IN DROUGHT PRONE AREA OF MAHARASHTRA (INDIA).

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The organochlorine compounds are manufactured since 1940 for use as pesticides. It is known that organochlorine insecticides easily accumulate and persist in living system. They are prepared commercially for use in the different fields in the form of dust, spray, liquids and wetable powder, which are generally used individuals and also in combination with other pesticides. Their extensive use during 1940-1970s revolutionized modern agriculture, which interns increased the output of crops. However, they are not safe for house hold applications as they persist in the environment for large duration after their initial use. The organochlorine, organophosphorous, pyrethroids etc. pesticides are widely used in agriculture. Their applications and usage have increased tremendously in the few last decade. Drought prone area of Maharashtra state (India) is famous for pomegranate and horticultural activities. To control crop pest and to improve crop yield various kinds of pesticides and fertilizers were applied on large scale Especially use of organochlorine pesticide is banned by many country because of their bioaccumulative properties in aquatic organisms and human health hazards, still they were used in drought prone area.

By considering these aspects present study was conducted to study health risk assessment, pesticides use and practices in drought prone area of Maharashtra (India).

PP 176

SELECTIVE EXTRACTION AND SPECTROPHOTOMETRIC DETERMINATION OF PLATINUM (IV) WITH 4-(2'-FURALIDENEIMINO)-3-METHYL-5-MERCAPTO-1, 2, 4-TRIAZOLE IN N-BUTANOL AND ITS APPLICATIONS TO REAL SAMPLES

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A simple, convenient, highly selective and sensitive extractive spectrophotometric procedure for determination of platinum(IV) has been developed by using 4-(2'-furalideneimino)-3-methyl-5-mercapto-1,2,4-triazole(FIMMT).The platinum (IV) forms red colored complex with FIMMT at pH 5.4 with 25 min heating in hot water bath. It is then extracted with n-butanol and has maximum absorbance at 510 nm with extinction coefficient 11686 L mol-1 cm-1 and Sandell's sensitivity 0.017 µg cm-2. The effect of pH, excess of reagent and foreign ions on the determination of platinum (IV) and the effect of heating time, stability and the solubility of complex with various solvents were studied. The method is precise and has been applied to the determination of platinum (IV) from synthetic matrices and also from real samples such as cis-platin injection and platinum–rhodium thermocouple wire. The method is well applicable for the group separation of platinum, palladium and nickel.