ISCBC-2011

15th International Conference on

Bridging Gaps in Discovery and Development : Chemical & Biological Sciences for Affordable Health, Wellness & Sustainability

04th - 07th, FEBRUARY 2011

Organized by

Indian Society of Chemists and Biologists
Lucknow

Saurashtra University
Rajkot

Co-Sponsored by

Department of Science & Technology
(DST - DPRP), New Delhi

Gujarat Council on
Science & Technology
Gandhinagar

INDIAN SOCIETY OF CHEMISTS & BIOLOGISTS

JOINTLY ORGANIZED BY

INDIAN SOCIETY OF CHEMISTS & BIOLOGISTS, LUCKNOW

DEPARTMENT OF CHEMISTRY SAURASHTRA UNIVERSITY, RAJKOT

PATRONS

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Saurashtra University, Rajkot, INDIA

Chief Patron

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Gov. of India, INDIA

Chief Patron

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Department of Science & Technology, INDIA

President & Organizing Scretary, ISCB

Prof. Anamik Shah

Department of Chemistry,
Saurashtra University, Rajkot, INDIA

General Secretary, ISCB

Dr. P.M.S. Chauhan,

ScientistF, Medicinal And Process Chemistry Div.
Central Drug Research Institute, Lucknow, INDIA

International Advisor, ISCB

Dr. Mukund S. Chorghade,

President & Chief Scientific Officer,
THINQ Pharma, Notick, MA-USA

Inaugural Function 3:45pm - 4:45pm

Inaugural Session

Opening Remrks By

Dr. Shailesh Ayyangar

Managing Director, Sanofi-Aventis India
Vice President - South Asia

05:00pm-PL-01

"Screenig for Biological Activity of Natural and Synthetic products in a laboratory of chemistry. Application to antibacterial agents"

Prof. Nicole J. Moreau

President, IUPAC (Intenational Union of Pure & Applied chemistry)
General Secretary CNC (Comite National de la Chimie)
Maison De la Chimie, Paris, France

05:30pm-PL-02

"25 Years of Carbon Nanomaterials : From Buckyballs to Graphene"

Prof. Luis Echegoyen,

Robert A. Welch Professor of Chemistry,
university of Taxes at El Paso Biosciences
University Ave., El Paso, TX-USA

06:00pm-PL-03

"Medicinal chemistry, an ever evolving discipline"

Prof. Henk Timmerman

Wijttenbachweg, Oegstgeest, The Netherlands

06:30pm-PL-04

"Cyclooligomerization : A simple way to complex structures"

Dr. Tushar Chakraborty

Director, Central Drug research Institute, (CDRI)
Lucknow, INDIA

POSTER PRESENTATION SESSION 1 TO 100
FOLLOWED BY DINNER

HALL - 1

08:45am-PL-05

"India Providing a Solution for Pharma R & D Productivity Issues" Beyond Cost Arbitrage and Other Common" Considerations"

Dr. Rashmi barbhaiya,
CEO & Managing Director, Advinus Therapeutics Ltd, Bangalore

09:15am-PL-06

"Hetrocuclic Chemistry At The Edge Of Biology And Medicine- The Past, Present, and Future Of Wsg1060"

Prof. Colin J. Suckling,
Freeland Professor of Chemistry, University of Strathclyde, Department of Pure & Applied Chemistry, Glasgow, Scotland

09:45am-PL-07

"Will India Ever Produce the First Indigenous New Drug for the global market ?"

Dr. B. K. Trivedi,
CSO, Medicinal Chemistry, Drug Discovery
Wockhardt R & D, Aurangabad, INDIA

10:15am-PL-08

"Opportunities and Challenges in Natural Product Synthesis for Drug Discovery"

Dr. J. S. Yadav
Director, Indian Institute Of Chemical technology, Hyderabad, INDIA

HALL - 2

08:45am-PL-13

"A new class of compounds showing a variegate reactivity and an interesting biological profile"

Prof. Domenico Spinelli,
University of Bologna, Italy

09:15am-PL-14

"Catalytic Reactions Access To Biologically Active Complex Molecules"

Prof. Gree Rene
Directeur de Recherche CNRS, Universite de Rennes
Sciences Chimiques de Renees, France

09:45am-PL-15

"Metal- Catalyzed C-H Bond Functionalizations for Sustainable Synthesis"

Prof. Luts Ackermann
Institut Fuer Organische and Biomolekulare Chemie
Georg-August-university of Goettingen, Tammannstr Goettingen (Germany)

10:15am-PL-16

"Single Use Biopharmaceutical Production technology - Green, Efficient and Sustainable Manufacturing"

Prof. Ronald Jordan
Dean, Department of Biomedical and Pharmaceutical Sciences, University of Rhode Island, USA

High Tea 10:45am to 11:05am

11:05am-PL-09

"Reverse Pharmacology and Systems Approaches for Chemical Biology"

Dr. Mukund S. Chorghade,
President & Chief Scientific Officer, THINQ Pharma, Natick, Ma-USA

11:35am-PL-10

"Synthesis and SAR of new glycyrrhetinic acid derived derivatives as 11β-hydroxysteroid dehydrogenase" inhibitors"

Prof. Ulrich Jordis
Vienna University of Technology, Inst. of Applied Synthetic Chemistry, getreidemarkt - Vienna, Austria

12:05pm-PL-11

"Human Pyruvate Dehydrogenase Complex : Structure-Function Relationship And Regulation"

Prof. Mulchand Patel
Department of Biochemistry, School of Medicine and Biomedical Sciences, University at Buffalo (UB), The State University of New York, USA

12:35pm-PL-12

"Isoform-selective inhibitors of PARP-2: Design, synthesis and evaluation"

Prof. Mike Threadgill
Department of Pharmacy & Pharmacology University of Bath, Claverton Down, Bath BA2 7AY, USA

11:05pm-PL-17

"Peptide Nanostructures as Molecular Transporters of Therepeutic Agents"

Prof. Keykavous Parang,
Medicinal Chemistry and Pharmacology,
Department of Biomedical Sciences, university of Rhode Island, USA

11:35am-PL-18

"Fabrication and the Applications of Hierachically Ordered Nano/ Macroporous Films and Powders"

Prof. Ajayan Vinu
Senior Scientist, NIMS ambassador (India) International Center for Materials Nanoarchitectonics World Premier International research Center National Institute for Materials Science, Tsukuba, Japan

12:05pm-PL-19

"Exporing the benefits of microwave irradition in heterocyclic chemistry"

Prof. Erik Van der Eycken
Katholieke Universiteit Leuven, Department of Chemistry
Laboratory for Organic and Microwave-Assisted Chemistry
Celestijnenlaan Belgium

12:35pm-PL-20

"complete Characterization of Protein-Based Biotherapeutics using Ultra-Performance Liquid Chromatography (UPLC) technology"

Dr. Dorothy Philips,
Director, Strategic Marketing
Waters Limited, MA USA

Lunch Time 01:05pm to 02:25pm

02:15pm-IL-01

"Metallic Saviour " Chemical and Biotechnological Develpments of Metal Based Macro to Nano chemotherapeutics"

Prof. Sartaj Tabassum
Div. Of Inorganic Chemistry, Department Of Chemistry,
Aligarh Muslim university, Aligarh

02:35pm-IL-02

"Collaborative Drug Discovery Efforts to Overcome the Gap Between Chemistry and Biology"

Dr. Raj Rajur,
Chairman & CEO, Creagen Bioscoences, USA

02:55pm-IL-03

"The De Novo Synthesis Of Biologically Important Natural Products And Carbohydrate Chemistry With Applicable To Medicinal Chemistry"

Prof. George O'Dohorty
North Eastern university
MA-USA

03:15pm-IL-04

"New Prespectives in cancer chemotherapeutic Drug Design : Effect of Metal ions, Ligand topology and chiral discrimination"

Prof. Farukh Arjamand,
Department Of Chemistry, Aligarh Muslim University, Aligarh

02:15pm-IL-05

"Synthesis and Antimicrobial Activity Evaluation of Cyclohexane-1,2-and 1,3-diamine Derivatives and Metronidazole-Triazole Conjugates"

Prof. Diwan Singh Rawal
Department Of Chemistry,
University of Delhi, Delhi, INDIA

02:35pm-IL-06

"Novel Conversion Of Multistep Reactions into Rapid One Pot MCR Under MWi For Syntheses Of Potentially Bioactive Heterocycles"

Prof. Kishor S. Jain,
Dean, Faculty of Pharmacy,
Sinhgadh College Of Pharmacy, Pune, INDIA

02:55pm-IL-07

"Bioactive Compounds from North American Maple (Acer) Species"

Prof. Navindra P. Seeram
Bioactive Botanical Research Laboratory, Department of Biomedical and Pharmaceutical Sciences, college of Pharmacy, University of Rhode Island, Kingston, RI, USA

03:15pm-IL-08

"Novel approaches to synthesis of new nitrogen, oxygen & sulphur heterocucles with potential medicinal significance"

Prof. Anjali rahatgaonkar,
Department Of Chemistry,
Institute Of Science, Nagpur, INDIA

Tea Break - 03:35pm - 03:50pm

Oral Presentations

03:50pm Oral Presentation-01
04:05pm Oral Presentation-02
04:25pm Oral Presentation-03
04:40pm Oral Presentation-04
04:55pm Oral Presentation-05

Oral Presentations

03:50pm Oral Presentation-06
04:00pm Oral Presentation-07
04:10pm Oral Presentation-08
04:20pm Oral Presentation-09
04:30pm Oral Presentation-10
04:40pm Oral Presentation-11
04:50pm Oral Presentation-12

POSTER PRESENTATION SESSION 101 TO 200

HALL - 1

8:45am-PL-21

"Discovery, optimization and mechanisms of action / resistance for novel antimalarial compounds"

Prof. Akhil B. Vaidya
Professor, Microbiology and Immunology
Director, Center for Molecular Parasitology
Drexel University College of Medicine, Philadelphia

09:15am-PL-22

"In search for novel and potent P-glycoprotein inhibitors as multidrug resistance reverting agents in cancer Chemotherapy"

Prof. Giampietro Sgaragli
University of Siena, Italy

09:45am-PL-23

"Avoiding Multidrug Resistance while Targeting Cancer Cells"

Prof. Paul Erhardt
University of Toledo, OHIO

10:15am-PL-24

"Catalyric Reactions Access to Biologically Active Complex Molecules"

Prof. Jannine Cossy
Professor of Organic Chemistry
Laboratoire de Chimie Organique, ESPCI Paris Tech, Vauquelin Paris

HALL - 2

08:45am-PL-29

"Novel Materials Involved in Radiological Environments"

Dr. Tina M. Nenoff
Distinguished Member of Technical Staff
Sandia National Laboratories, Albuqueque, NM, USA

09:15am-PL-30

"Health informatics : The NPU Coding System"

Dr. Francoise Pontet
(On behalf of the Joint IFCC-IUPAC Committee on Nomenclature for Properties and Units)
Service de Biochimie et Biologie Moleculaire, Hospital Lariboisiere, 2 rue A Pare, Paris, France.

09:45am-PL-31

"Synthesis Tool Compounds for Chemical Biology"

Prof. Rolf Breinbauer
Institute of Organic Chemistry, Graz University of Technology, Graz, Austrelia.

10:15am-PL-32

"Synthesis of Fty 720 And Novel C-Glycosylated Phenstatin Analogues Using Weinreb Amide Based Building Blocks"

Prof. Indrapal Singh Aidhen
Department of Chemistry,
Indian Institute of Technology Madras, Chennai, INDIA

High Tea 10:45am to 11:05am

11:05pm-PL-25

"Isocyanide based multi component reactions for heterocyclic synthesis"

Prof. Laurent El Kaim
Enseignant-Chercheur, DCSO (Ecole Polytechnique)
ENSTA
Paris (France)

11:35pm-PL-26

"Chemistry, biology of novel anti-inflammatory and anti-cancer agents"

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

12:05pm-PL-27

"Molecular Diversity through Design and Development of New Reactions Based on Novel Organosulfur Synthons."

Prof. H. Ila
INSA Senior Scientist,
Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, INDIA

12:35pm-PL-28

"Aromatic and Hetro aromatic Annulation, Universal Synthetic Strategy for Benzo and Condensed Heterocycles"

Prof. H. Junjappa
Reva Institute of Science & Management,
Bangalore, INDIA

11:05pm-PL-33

"De Novo Synthesis of Carbohydrates"

Prof. Graham Jones
Bioorganic and Medicinal Chemistry, Department, Chair,
Department of Chemistry & Chemical Biology
Northeastern University, Huntington Ave, Boston, Massachusetts, USA

11:35am-PL-34

"Using Chemistry to Bridge Gaps Between Nations"

Dr. Zafra Lerman
President, MIMSAD Inc., Evanston IL, USA

12:05pm-PL-35

"Proteomics of Hepatitis C Virus - Host Cell Interaction : Identification of cellular / viral factors associated with HCV (+) strand RNA Genome"

Prof. Virendra N. Pandey
Department of Biochemistry and Molecular Biology,
New Jersey Medical School, UMDNJ, Newark, NJ USA

12:35pm-PL-36

"Discovery of therapeutics for the spinocerebellar ataxia type 1 (SCA1)"

Prof. Ramaiah Muthyala
Associate Director, Center for Orphan Drug Development
Associate Professor, Department of Clinical Pharmacology & Department of Medicinal Chemistry, Adjunct Professor, Department of Medicine, University of Minnesota, Minneapolis, MN USA

Lunch Time - 01:05pm to 02:05pm

HALL - 1

02:15pm-IL-09

"Target repurposing for neglected tropical disease drug discovery"

Dr. Michael Pollastri
Associate Professor, Medicinal Chemistry and Chemical Technology, Department of Chemistry & Chemical Biology
417 Egan Research Center, Northeastern University, USA

02:35pm-IL-10

"Sustainable and Greener Methodology Development for the Synthesis of Nucleosides of Importance in Healthcare."

Prof. Ashok K. Prasad
Department of Chemistry, University of Delhi, Delhi.

02:55pm-IL-11

"Designing a Green Reaction"

Prof. Brindaban C. Ranu
Indian Association for the Cultivation of Science.

03:15pm-IL-12

"A systematic study of benzimidazoles in search of selective antimicrobials targeting topoisomerase I : Development of E.coli. Inhibitors"

Dr. Vibha Tondon
Associate Professor, Department of Chemistry
University of Delhi

HALL - 2

02:15pm-IL-13

"Environmentally sustainable technique for production of bioactive compounds from agriculture wastes."

Dr. Brajesh Kumar
Assistant Professor, Department of Molecular Biotech,
School of Life & Environmental Science, Konkuk University, Korea

02:35pm-IL-14

"Fundamental Research Leading to Rational Synthesis of Novel MIF Antagonists For Mitigating Auto-Immune / Inflammatory Disorders"

Dr. Nilesh Dagia
Department of Pharmacology,
Group Leader,
Piramal Life Sciences Limited, Mumbai

02:55pm-IL-15

"Tandem Synthesis of Indolo-, Pyrrolo (2,1-a) isoquinolines, Naphthyridines, Pyranoquinolines, Pyranoquinolinones and Isocumarins by the Electrophilic Cyclization of Alkanes"

Dr. Akhilesh K. Verma
Associate Professor, Dept. of Chemistry,
University of Delhi, Delhi.

03:15pm-IL-16

"Pyrazolo (3,4-d) pyrimidine core as novel system for studying arene Interactions in flexible polyethylene linker compounds especially propylene linker compounds."

Dr. K. Avasthi
Scientist F, Medicinal And Process Chemistry Division, Central Drug Research Institute, Lucknow

Tea Break - 03:35pm to 03:50pm

AWARDS

03:50pm

ISCB AWARD FOR EXCELLENCE-2011
CHEMICAL SCIENCES

Prof. Katsuhiko Ariga
Director & Principal Investigator, World Premier International (WPI)
Research Center for Materials Nanoarchitectonics (MANA)
National Institute for Materials Science (NIMS), JAPAN

04:20pm

ISCB AWARD FOR EXCELLENCE-2011
CHEMICAL SCIENCES

Prof. Krishna Kumar
Chairman, Department of Chemistry,
Tufts University, Medford, MA

04:50pm

ISCB DISTINGUISHED WOMEN SCIENTIST AWARD

Dr. Rukhsana I. Kureshy
Scientist - EII, Central Salt and Marine Chemicals
Research Institute (CSMCRI), Bhavnagar, Guj-INDIA.

05:05pm

ISCB YOUNG SICENTIST AWARD
CHEMICAL SCIENCES

Dr. Partha Sarathi Mukherjee
Inorganic & Physical Chemistry Department,
Indian Institute of Science, Bangalore.

05:20pm

ISCB YOUNG SCIENTIST AWARD
BIOLOGICAL SCIENCES

Dr. Vikash Kumar Dubey
Associate Professor, Department of Biotechnology,
Indian Institute of Technology Guwahati, Assam, India.

Poster Presentation Session 201 onwards

HALL - 1

08:45am-PL-37

"Motivational tools in challenging olefin metathesis reactions"

Prof. Karol Grela
Institute of Organic Chemistry, Polish Academy of Sciences, Organometallic Synthesis Laboratory, Faculty of Chemistry, University of Warsaw, Warsaw, Poland.

09:15am-PL-38

"Application of Catalysts in Synthesis of Heterocyclic Compounds"

Prof. P. T. Perumal
Head & Scientist 'G', Organic Chemistry Division, Central Leather Research Institute, Chennai INDIA

09:45am-PL-39

"Natural products-based (from Piper & Tephrosia species) anti-mocribal, anti-inflammatory and antiplatelet agents"

Prof. V. S. Parmar
Professor of Organic Chemistry,
Department of Chemistry, University of Delhi, Delhi-INDIA.

10:15am-PL-40

"A Modular Approach To Chiral Imidates: A New Class of Nitrogen-Based Chiral Ligands."

Prof. Johan Van der Eycken
Laboratory for Organic and Bioorganic Synthesis, Department of Chemistry, Ghent University, Belgium

HALL - 2

08:45am-PL-45

"Developing Drugs for Complex Diseases: Understanding the Clinical Need"

Dr. Michael Liebman
President / Managing Director, Strategic Medicine, Inc
PA USA

09:15am-PL-46

"First & Second Generation Paratransgenics : Tools for the Control of Global vector for Borne Diseases"

Prof. Ravi Durvasula
MD, Chief of Medicine and Acting ACOS for Research,
New Maxico VA Health Care System
Vice Chairman for VA Affairs and Director, Center for Global Health, Dept of Internal Medicine, USA

09:45am-PL-47

"Health and wellness by natural products and Neutraceuticals"

Dr. K. P. Mohanakumar
Head & Scientist-G, Cell Biology & Physiology Division,
Indian Institute of Chemical Biology, Calcutta, INDIA

10:15am-PL-48

"Ajulemic Acid: A Novel CB 1/2 Agonist for Neuropathic Pain"

Dr. Kollol Pal
CEO, Mnemosyne Pharmaceuticals Inc, USA

High Tea 10:45am to 11:05am

11:05am-PL-41

"Efficient Approach To Heterocyclic"

Prof. Dong-Soo shin
Department of Chemistry, Changwon National University#9 Sarimdong, Changwon, Kyongnam, 641-773, S. Korea

11:35pam-PL-42

"TNF-ALFA Inhibitors Potentially Active Against Mycobacterium Sp"

Prof. Chung Man Chin
LAPDESF - Laboratory of Drug Design. Department of Drugs and Medicines - School of Pharmaceutical Sciences - University of Sao Paulo State - UNESP, Araraquara, SP, BRAZIL

12:05pm-PL-43

"Synthesis of Novel 3,4-Diaryll-1,2,4 Triazoles As Well As 2-Substituted Thiazolo (4,5-F) Isoquinolines / Quinolines And Benzo(1,2-D: 4,3-D) Bisthiazoles As Potent Cox-1/2 Inhibitors"

Prof. Athina Geronikaki
Head of the laboratory of Pharm. Chemistry
School of Pharmacy, Aristotle University
of Thessaloniki, Thessaloniki 54124, Greece

12:35pm-PL-44

"Synthesis of Novel Heterocyclic Compounds for Induction of Apopotosis in Human Leukemia Cells"

Prof. K. S. Rangappa
Vice-Chancellor, Karnataka State Open University (Ksou), Mysore

11:05pm-PL-49

"Identifying residue-specific contributions to protein stability and stabilization"

Dr. Jenifer Laurense
Associate Professor, Pharmaceutical Chemistry, University of Kansas USA

11:35pm-PL-50

"NO donating hybrid molecules - a chance to improve the therapy of Alzheimer's disease"

Prof. Jochen Lehmann
Chair holder of Pharmaceutical / Medicinal Chemistry,
Institute of Pharmacy, University of Jena
Philosophenweg, Jena, Germany

03:45pm-PL-51

"Design and Synthesis of Thiazolidine - 4 - ones new Antihyperglycaemic Agents"

Dr. S. B. Katti
Scientist G, Medicinal & Process Chemistry Division, Central Drug Research Institute, Lucknow, INDIA

02:45pm-PL-52

"Design Strategies Targeting Type II and Allosteric Sites: New Trends and Opportunities beyond Type I Kinase Domain Site."

Prof. Hariprasad Vankayalapati
Chief Scientist, Medicinal Chemistry,
Centre for Investigational Theraputics, Hunstman Cancer Institute,
Salt Lake City, USA

Lunch Time 01:05pm - 02:05pm

HALL - 1

02:15pm-IL-17

"Chiron Approach Synthesis of Natural Products and Natural Product like molecules from carbohydrate-based building blocks"

Prof. A. K. Shaw
Scintist F, Medicinal And Process Chemistry Division,
Central Drug research Institute, Lucknow INDIA
Aligarh Muslim university, Aligarh

02:35pm-IL-18

"Design and Synthesis of Nitrogen Heterocycles as Novel Therapeutic Agents"

Dr. P.M.S. Chauhan,
Scintist F, Medicinal And Process Chemistry Division,
Central Drug Research Institute, Lucknow INDIA

02:55pm-IL-19

"Indolyl azoles as Novel and Selective Anticancer Agents"

Prof. Dalip Kumar
Group Leader Chemistry Group, BITS, Pilani, Rajasthan, INDIA

03:15pm-IL-20

"Discovery of NCEs at Saurashtra University"

Prof. Anamik Shah,
Professor & Principal Investgator
National Facility of Drug Discovery
Department of Chemistry Saurashtra university, Rajkot INDIA

HALL - 2

02:15pm-IL-21

"Paptide-Oligonucleotide Conjugate as Therapeutics"

Dr. W. Haq
Scientist F, Medicinal And Process Chemistry Division,
Central Drug Research Institute, Lucknow

02:35pm-IL-22

"Role of Organic Chemistry in Healthcare : An Industrial Perspective"

Dr. Rakeshwar Bandichor,
Senior Scientist, Dr. Reddy's Laboratories Ltd.,
Hyderabad

02:55pm-IL-23

"4-Oxo-thiazolidines: Important Scaffolds in the new millennium for the development in pharmaceutical industries"

Prof. N. C. Desai,
Head, Department of Chemistry,
bhavnagar University, Bhavnagar, INDIA

03:15pm-IL-24

"Novel Substituted 1H-benzol[d]imidazole-2-carboxamide derivatives as selective and oral CB2 agonists for the prevention of allodynia in rat neuropathic pain models"

Dr. Brijesh Srivastava
Zydus Research Center.
Ahmedabad, Gujarat

Tea Break - 03:15pm - 03:50pm

RSC - PTG & ISCB BEST POSTER EVENT

VALEDICTORY FUNCTION

Her Excellency, The Governor of Gujarat,
DR. SHRIMATI KAMLA
Will Grace The Valedictory Function.

DR. SHRIMATI KAMLA
Her Excellency,
Governor of Gujarat,
Gandhinagar

Date : 7th February 2011, Monday
Time : 04:00pm to 05:30pm
Place : Hotel The Grand Bhagavati Seasons,
Kalawad Road, Rajkot.

Local Organizing Committee

Co-Chair Person: Dr. G. C. Bhimani, Dean-Science Faculty, Saurashtra University
Convener: Dr. P. H. Parsania, Professor & Head, Department of Chemistry, Saurashtra University
Co-Convener: Dr. H. S. Joshi, Professor, Department of Chemistry, Saurashtra University

Shri G. M. Jani, Registrar, Saurashtra University
Dr. V. H. Shah, Professor, Department of Chemistry, Saurashtra University
Dr. S. H. Baluja, Professor, Department of Chemistry, Saurashtra University
Dr. U. C. Bhoya, Asso. Professor, Department of Chemistry, Saurashtra University
Dr. M. K. Shah, Asst. Professor, Department of Chemistry, Saurashtra University
Dr. Y. T. Naliapara, Asst. Professor, Department of Chemistry, Saurashtra University
Dr. R. C. Khunt, Department of Chemistry, Saurashtra University
Dr. N. R. Sheth, Professor & Head, Department of Pharmaceutical Science, Saurashtra University
Dr. P. P. Sood, Former Professor & Head, Department of Bioscience, Saurashtra University
Dr. S. P. Singh, Professor & Head, Department of Bioscience, Saurashtra University
Dr. V. S. Thaker, Professor, Department of Bioscience, Saurashtra University
Dr. Nilambari Dave, Asso. Professor & Head, Department of Home Science, Saurashtra University
Dr. K. N. Iyer, Professor & Head, Department of Physics, Saurashtra University
Dr. D. G. Kuberkar, Professor, Department of Physics, Saurashtra University
Dr. M. J. Joshi, Professor, Department of Physics, Saurashtra University
Dr. H. P. Joshi, Professor, Department of Physics, Saurashtra University
Dr. N. A. Shah, Asst. Professor, Department of Electronics, Saurashtra University
Dr. M. N. Jivani, Asst. Professor, Department of Electronics, Saurashtra University
Dr. C. M. Kanabar, Technical Assistant, Department of Computer Science, Saurashtra University
Dr. C. K. Kumbharana, I/C Head, Department of Computer Science, Saurashtra University
Dr. Bhadrayu Vachhrajani, Academic Staff College, Saurashtra University
Dr. Kaladhar Arya, Academic Staff College, Saurashtra University
Mr. Nilesh Soni, Chief Librarian, Saurashtra University
Mr. N. V. Jobanputra, Computer Center, Saurashtra University
Mr. K. N. Kher, Chief Accountant, Saurashtra University
Dr. Kalpesh Ganatra, Principal, Shri M V M Science College, Rajkot
Dr. Y. Fernandes, Head – Department of Chemistry, Christ College, Rajkot
Dr. A. U. Patel, Principal, Shri M & N Virani Science College, Rajkot
Dr. K. D. Ladva, Head – Department of Chemistry, Shri M & N Virani Science College, Rajkot
Dr. S. K. Joshi, H & H B Kotak Science College, Rajkot

TASK COMMITTEE

No	Committee	Coordinator	Members	
	Chairperson of the Task Committee: Dr. P. H. Parsania, Professor & Head, Department of Chemistry, Rajkot			
1	Abstract & Souvenir	Dr. Anamik Shah Dr. Tushar Mehta	Mr. Pratik Ambasana	Mr. Dilip Detroja
2	Accommodation	Mr. Punit Rasadiya	Mr. Bharat Savaliya Mr. Harshad Kaila Mr. Bhavin Marvaniya Mr. Bhavesh Dodiya Mr. Renish Ghetiya	Dr. Mahesh Savant Mr. Vipul Audichya Mr. Dipak Vachhani Mr. Gaurang Pandya
3	Accounts	Mr. Hardevsinh Vala	Mr. Krunal Mehariya Mr. Harshad Joshi	Mr. Shailesh Parekh Mr. Dilip Detroja
4	Advertisement	Dr. Anamik Shah	Mr. Abhay Bavishi	Mr. Shailesh Thakrar
5	Computer Support	Dr. Manish Shah Dr. S. K. Joshi	Mr. Ashish Radadiya Mr. Ravi Chaniyara Mr. Dilip Detroja	Mr. Vaibhav Ramani Mr. Rizvan Ghumara Mr. Suresh Koradiya
6	Cultural Event	Dr. Shipra Baluja Dr. Falguni Karia Dr. Ranjan Khunt Dr. Valentina Umraniya	Ms. Leena Joshi MS. Chetana Rajyaguru MS. Rekhabaa Jadeja	Ms. Minaxi Maru Dr. Bhavana Vaidya Ms. Manisha Parmar
7	ISCB Secretariat Team	Dr. Anamik Shah	Mr. Dilip Detroja Ms. Vishwa Dhinoja Mr. Punit Rasadiya Mr. Bharat Savaliya Mr. Vaibhav Ramani Mr. Ashish Radadiya Mr. Dhairya Bhavsar Mr. Shrey Parekh Mr. Shailesh Thakrar Mr. Nilay Pandya	Mr. Pratik Ambasana Ms. Ketaki Chauhan Mr. Krunal Mehariya Mr. Hardev Vala Mr. Abhay Bavishi Ms. Manisha Parmar Mr. Mrunal Ambasana Mr. Harshad Kaila Mr. Hitesh Sarvaia Mr. Rakshit Thakkar
8	Poster Presentation	Dr. Hitendra Joshi Dr. Shipra Baluja Dr. Ranjan Khunt Dr. Deenish Karia	Mr. Hardev Vala Mr. Pratik Ambasana Mr. Govind Kher	Ms. Manisha Parmar Mr. Bharat Bhuva Mr. Piyush Vekariya
9	Press & Publicity	Dr. Anamik Shah Dr. Kartik Ladwa Dr. D. M. Purohit	Mr. Dhairya Bhavsar Mr. Shrey Parekh	Mr. Shailesh Thakrar
10	Reception & Registration	Dr. U. C. Bhoya Dr. Ranjan Khunt Dr. Falguni Karia Ms. Y. Fernades	Ms. Vishwa Dhinoja Mrs. Pooja Parsania Ms. Leena Joshi Ms. Ketaki Chauhan Ms. Manisha Parmar Mr. Hitesh Sarvaia	Mr. Paresh Ladwa Mr. Ashish Patel Mr. Gaurang Pandya Mr. Shrey Parekh Mr. Jignesh Patel Mr. Rakesh Tada
11	Scientific Session	Dr. PMS Chauhan Dr. W. Haq Dr. Mukund Charghade	Dr. H. S. Joshi Dr. V. H. Shah Dr. S. H. Baluja	Dr. Y. T. Naliapara Dr. M. K. Shah Dr. U. C. Bhoya
12	Tour Arrangement	Dr. Manish Shah Dr. Denish Karia Dr. Jatin Upadhyay	Mr. Hitesh Sarvaiya Mr. Ritesh Bhatt	Mr. Naimish Chavda
13	Transportation	Dr. Yogesh Naliapara Dr. Viresh Shah Dr. Denish Karia	Mr. Piyush Pipaliya Mr. Mrunal Ambasana Mr. Amit Trivedi Mr. Shailesh Thakrar	Mr. Anil Patel Mr. Vaibhav Ramani Mr. Punit Rasadiya Mr. Bharat Savaliya Mr. Ritesh Bhatt
14	Video Recording & Documentation	Dr. C. K. Kumbharana Dr. C. M. Kanabar	Mr. Pratik Dave Mr. Mrunal Ambasana	Mr. Yashvant Jadeja

Massage from VC

It is a matter of great pleasure to welcome the scientists from various countries across the globe and delegates from Industries, Universities and other research institutes from India for ISCBC-2011, one of the major happening of science at this wonderful city, Rajkot.

Saurashtra University is a State level University having 27 postgraduate departments and 343 affiliated colleges covering almost 2,000,000 students from various faculties with 238 academic programs of undergraduate, postgraduate and doctoral programme, is spearheading a sea change in recent years in terms of infrastructure, curriculum, diversity of courses addressing local need and pursuing for global standards. The faculty of science and especially Department of Chemistry, Department of Biosciences, and Department of Physics are known for their high academic and research output with India and abroad. They are recognized by several agencies like University Grant Commission, New Delhi (UGC), and also under Fund for Improvement of Science and Technology, New Delhi (FIST).

I'm happy that Indian Society of Chemist and Biologist (ISCB) has decided Rajkot as venue for this International event after a long break of almost six years.

I must congratulate the faculty of department of Chemistry for their untried efforts from months to organize such a mega event in the Saurashtra University and especially to Prof. P.H. Parsania, Prof. Anamik Shah and their research team to take a lead to organize this conference. I hope that we will receive the fruits of this conference in terms of greater contribution to the scientific community by young scientist for the development of science in the coming years.

I'm sure that young generation from different part of India who are present here in large numbers will be enjoying our Saurashtrian hospitality, culture events especially planned for our guests and delegates.

Congratulations!

सत्यमेव जयते
डॉ.टी.रामसामी
सचिव
Dr. T. RAMASAMI
SECRETARY

भारत सरकार
विज्ञान और प्रौद्योगिकी मंत्रालय
विज्ञान और प्रौद्योगिकी विभाग
टेक्नोलाजी भवन, नया महरौली मार्ग, नई दिल्ली-110 016
GOVERNMENT OF INDIA
MINISTRY OF SCIENCE & TECHNOLOGY
DEPARTMENT OF SCIENCE & TECHNOLOGY
Technology Bhavan, New Mehrauli Road, New Delhi-110 016

MESSAGE

I am delighted that Indian Society of Chemists and Biologists (ISCB) and Saurashtra University are jointly organizing an International Conference at Rajkot on February 4-7, 2011 on one of the important themes of contemporary relevance. The steps for reducing the gap between discovery and development of a drug are many and merit closer scientific scrutiny. I look forward to some implementable recommendations emanating from the Conference. In the "International Year of Chemistry", let me wish that this Conference serves to bridge cross-boundary interactions between chemistry and biology.

I wish the event a grand success.

(T Ramasami)

प्रो. समीर के. ब्रह्मचारी
महानिदेशक, वै.औ.अ.प.
एवं सचिव, भारत सरकार
वैज्ञानिक और औद्योगिक अनुसंधान विभाग

Prof. Samir K. Brahmachari
Director General, CSIR
& Secretary, Government of India
Department of Scientific & Industrial Research

वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद्
अनुसंधान भवन, 2, रफी मार्ग, नई दिल्ली-110001
COUNCIL OF SCIENTIFIC & INDUSTRIAL RESEARCH
Anusandhan Bhawan, 2, Rafi Marg, New Delhi-110001

MESSAGE

It gives me great pleasure to learn that the Department of Chemistry, Saurashtra University, Rajkot ,and the Indian Society of Chemists and Biologists are jointly organizing the 15th ISCB International Conference on "*Bridging Gaps in Discovery and Development: Chemical and Biological Sciences for Affordable Health, Wellness and Sustainability,*" during 04-07 February 2011.

Advances in genome analysis are increasing the number of potential drug targets as well as candidate molecules isolated from the Earth's biodiversity basket. Chemogenomics is now an emerging field. Simultaneously, tremendous advances in the field of chemistry have allowed synthetic pathways and molecules to be mimicked, thus paving the way for a more sustainable utilization of global resources. These developments mean that the pharmaceutical industry is currently poised on the verge of explosive growth. Affordable health is a human right that cannot be ignored and inexpensive drugs developed in a sustainable manner are the need of the hour. It is in this context that the 15th ISCB International Conference deserves appreciation.

It is extremely commendable that the 15th ISCB International Conference has been organized with the object of exchanging knowledge and skills relevant to the burning issues of affordable health and sustainability. I am certain that it will prove to be the perfect platform for experts to evolve strategies for implementing successful practices for affordable health and wellness in a sustainable manner on a global scale.

I wish the 15th ISCB International Conference on "*Bridging Gaps in Discovery and Development: Chemical and Biological Sciences for Affordable Health, Wellness and Sustainability,*" all success and congratulate the organizers on this timely initiative.

[Samir K Brahmachari]

New Delhi

December 9, 2010

सुखदेव थोरात
अध्यक्ष
Sukhadeo Thorat
Chairman

विश्वविद्यालय अनुदान आयोग
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December 06, 2010

MESSAGE

9 NOV 2010

I am extremely happy to know that the Department of Chemistry, Saurashtra University, Rajkot in association with the Indian Society of Chemists & Biologists is organizing an International Conference on "Bridging Gaps in Discovery and Development : Chemical and Biological Sciences for Affordable Health, Wellness and Sustainability" during February 04-07, 2011. Organizing the Conference on any topic is the only way to exchange the thoughts, I am sure that through this Conference, the University/Society will definitely be able to go ahead in this area. Releasing of the Souvenir on this occasion is also a good step of the University/Society to depict its policies/achievements etc.

I extend my best wishes and greetings to the University/Society for organizing such a Conference. I wish for the grand success.

(Sukhadeo Thorat)

Dr. Anamik Shah
Organizing Secretary
Department of Chemistry
Saurashtra University
Rajkot – 360 005 (Gujarat).

website
www.iscbindia.org

Indian Society of Chemists & Biologists

15th ISCB International Conference

4th - 7th February 2011

at Department of Chemistry Saurashtra University, Rajkot - 360 005.

President : Prof. Anamik Shah

General Secretary : Dr. P. M. S. Chauhan

ISCB PRESIDENT'S MESSAGE

I am very happy to welcome the dignitaries and delegates from many scientific forums, Universities, Research Organisations and pharmaceutical industries in the historical area of Saurashtra especially the wonderful city of Rajkot.

15th ISCB-2011 international conference with it's theme "Bridging Gaps in Discovery and Development: Chemical and Biological Sciences for Affordable Health, Wellness and Sustainability" is jointly hosted by Saurashtra University and Indian Society of Chemist and Biologist (ISCB), Central Drug Research Institute, Lucknow (CDRI).

Indian Society of Chemists and Biologists, Lucknow is an unique organization of dedicated researchers, scientists, academician and opinion leaders which was founded 15 years ago with a view to convene, sustain, support and extend the horizon of knowledge of several premier institutes of India to the remote places where quest for science & thirst for knowledge is the real want.

The Department of Chemistry of Saurashtra University, at Rajkot campus was founded in 1979 and I had the privilege to be the FIRST Doctorate from this campus under the guidance of the Founder & Head, Late Professor V.M. Thakor which has now become an excellent centre of learning in Chemistry especially Synthetic & Medicinal Chemistry (FIST funded & UGC Special Assistance Program) and is accredited B grade by NAAC.

The conference cannot be successful without eminent speakers and learners. I am very happy that the delegates present here has a specific role in the conference either as plenary speakers or an invited speakers, oral or as a Poster presenter.

Over the past several months, we have recieved overwhelming support from various Government agencies and Pharmaceutical companies. As President of ISCB & Organizing Secretary, I am thankful to GUSCOST, DST, ICMR, CSIR, Indian Pharmaceutical Companies and other industries, organizations and individuals who have generously helped organizers to make this conference a mega event.

Year 2011 has been declared as the year of Chemistry by IUPAC. Let all of us unite to agglomerate this wonderful science with rest of the branches & make the mother earth more beautiful by new innovations and strategies for clean and green technologies.

Anamik Shah

Prof. Anamik Shah

website
www.iscbindia.org

Indian Society of Chemists & Biologists

15th ISCB International Conference

4th - 7th February 2011

at Department of Chemistry Saurashtra University, Rajkot - 360 005.

President : Prof. Anamik Shah

General Secretary : Dr. P. M. S. Chauhan

Message from General Secretary, Dr.P.M.S.Chauhan

It is with immense pleasure that the scientific committee is bringing out this book of abstracts of scientific Programmers & Presentations to be made in 15th International Conference of Indian Society of Chemists and Biologists, CDRI lucknow, with a focused theme of ***"Bridging Gaps in Discovery and Development: Chemical and Biological Sciences for Affordable Health, Wellness and Sustainability"*** jointly organized by ISCB, Lucknow and Department of Chemistry, Saurashtra University, Rajkot. A close interaction between the scientist and technologists in the area of chemistry and biology is highly desired. With this view in mind, Indian Society Chemists and Biologists is making consistent efforts to encourage interdisciplinary research activities in the field of chemistry and biology.

I am happy that an extensive and comprehensive programme is arranged where thematic plenary, invited papers to be presented by eminent scientist blend intimately with the presentation of original research findings of young scientists, researchers and other professionals.

This comprehensive intentional programme, besides Inaugural function, includes 52 Plenary Lecturers, 24 Invited Lecturers, 15 Oral Presentations, and more than 300 Poster Presentations. Indin Society of Chemists & Biologists has achieved a prominent status in its 15 International Conference looking to the galaxy of speakers who made this conference an International event, for all four days. More than 700 participants are registered all over the country and across the globe. There is a scientific exhibition for the benefits of delegates.

I warmly welcome all National & International Speakers, guests and delegates from pharmaceutical companies and research organizations, universities and other academic institutes and wish them a very happy stay at this historical city of Rajkot. We wish that the message of this conference will spread through out India and other International Scientific Community as well.

We are thankful to the Vice Chancellor of Saurashtra University and officials of University and especially the faculty of Department of Chemistry and ISCB office bearers to arrange ISCB-2011 in a very grand way and for their utmost cooperation at every stage of conference. I'm also thankful to Dr. Mukund Chorghade for coordinating with galaxy of speakers from various parts of county.

Wishing all you a very happy new year!

PMSChauhan

Dr. PMS Chauhan

Pro. Vasuben Trivedi

MOS./Hi.Edu. & W.&C. Dev./ /337/2010.
Phone : 079-232 50188, 232 50195, 232 50189 (Fax)
Minister of State,
Higher & Technical Education,
Women & Child Development
Block No. 2/7, Sachivalaya Complex,
Gandhinagar (GUJ)-382 010
Date :- - 3 DEC 2010

It is a matter of pleasure that Indian Society of Chemists & Biologists "ISCB" & Saurashtra University, Rajkot are jointly organizing 15th International Conference on 4th - 7th Feb. 2011 on the Scientific theme of "Bridging Gaps in Discovery and Development: Chemical & Biological Sciences for affordable Health, Wellness and Sustainability."

Gujarat is the hub of Pharmaceutical industries. It is the need of hour that every industry should update in research & development to make pace with global competitors. In this era of jet-speed life style people are becoming more awaken about healthcare & wellness. Being aware of the side-effects of allopathic medicines, people are diverted to Natural & Ayurvedic system of medicine.

I congratulate you all, for compiling all above points in the theme of your conference. I hope it will help Gujarat especially in the field of Pharmaceutical, Neutraceutical, Chemical and Drug Industry. Organizing such an International conference in the year of "Swarnim Gujarat" celebrations and "International year of Chemistry – 2011" is a nice and appreciable gesture. I convey my best wishes for the success of conference & your sincere efforts.

(Prof. Vasuben Trivedi)

To,
Prof. Anamik Shah
Organizing Secretary – Indian Society of Chemists & Biologist Department of Chemistry Saurashtra University, Rajkot
Rajkot

Resi. :-Bunglow No. 5, Minister's enclave, Sector No. : 20, Gandhinagar-382 020
Phone : 079-232 32453.
Website : www.Prof Vasubentrivedi.com. Email :-mos-hiedu@gujarat.gov.in

PL - 01

Plenary Lectures

Prof. Nicole Jeanne Moreau

UMR 7573 CNRS – ENSCP Laboratoire de Synthèse sélective organique & produits naturels – Biochimie & criblage de molécules – Paris

After ten years of reseach in organic synthesis (terpenes, steroïds & sugars), Nicole J. Moreau successfully designed the 1st purification of enzymes that inactivate aminoglycoside antibiotics. Her research is at the interface of chemistry and life sciences, mainly in the field of antibacterial agents. She developed a medium throughput screening system in order to find molecules, from natural substances or synthesis, able to be active against resistant bacteria.

Professor Moreau received an M.S. in physical chemistry then a doctorate in physical sciences (chemistry distinction) from Paris XI University. She worked as a Research Director at CNRS, then as a professor at Paris 6 University and the Ecole Nationale Superieure de Chimie de Paris.

She has held a number of leadership positions with leading chemistry institutions. She has been Deputy Director of the Chemistry Department of CNRS, and is currently President of IUPAC (International Union of Pure & Applied Chemistry).

PL - 01

Plenary Lectures

Screening for biological activity of natural and synthetic products in a laboratory of chemistry. Application to antibacterial agents

Nicole J. Moreau*, Jean-Marc Paris, Pascale Bouhours & Carine Ganem-Elbaz
UMR 7573 CNRS – ENSCP Laboratoire de Synthèse sélective organique & produits naturels – Biochimie & criblage de molécules – Paris

ABSTRACT

In a laboratory of organic chemistry, people are supposed to synthesize or extract products, design new reactions, but not to assay for biological activity of their molecules or extracts. However, all the compounds synthesized or extracted constitute a non-exploited source of potentially active molecules.

In France, there is in the CNRS (National Centre for Scientific Research) about 100 laboratories more or less implied in extraction or synthesis, and if each of them prepares or extracts from 10 to 100 substances each year, there are from 1 000 to 10 000 compounds sleeping in drawers. We also have access to many French –and foreign- spots where there is a high biodiversity. To make use of all these compounds, the CNRS decided a few years ago to organize a national library of synthetic compounds and of natural extracts and pure molecules called the "Chimiothèque Nationale". The collect and storage of samples were homogeneous within all laboratories. This library constitutes a reservoir of potentially active compounds:

On another hand, chemists could be interested in assaying by themselves their products. This permit to avoid loosing time through transfer of products and results between teams of different disciplines, and as such be able to accelerate the process of discovery of potentially active molecules. But this is also for some chemists, and not only the youngest of them, an opportunity to learn new techniques and to diversify their area of interest.

PL - 03

Plenary Lectures

Prof. Henk Timmerman

VU University Amsterdam

Henk Timmerman(1937) received his Ph. D. of the Vrije Universiteit Amsterdam in 1967.Until 1979 he was employed by the pharmaceutical industry, first in research and later in a management function.In1979 he returned to his alma mater to succeed his PhD supervisor(Wijbe Th. Nauta) on the chair of Pharmacochemistry. In 2002 he had to retire from his professorship.

His research deals mainly with the medicinal chemistry and pharmacology of histamine receptors and their ligands. He is (co-) author of around 500 scientific papers including several book chapters. He supervised more than 40 Ph.D.programmes, among which there are several at Indonesian universities.

Henk Timmerman has had and has a number of positions at different scientific societies, both national and international. He was e.g. president of the Royal Netherlands Chemical Society, president of the Dutch Society for Pharmaceutical Sciences, member of the board of the Dutch Federation for Innovative Medicines Research, secretary and subsequently president of the European Federation of Medicinal Chemistry and member of DivisionVII of the IUPAC on Chemistry and Human Health.

He has been –or is- on the advisory board of several journals such as JMC and TIPS; currently he is editor of Drug Research Today – Technologies.

Among his honors are the Ariëns Prize for Pharmacology, The Nauta Award for Medicinal Chemistry, the Dr. Saal van Zwanenberg – Organon Medal for Pharmaceutical Sciences and the honorary membership of the Royal Netherlands Chemical Society as well as of The Dutch Pharmacological society. He received honorary doctorates from the Gadjah Mada University(Indonesia), the Medical University of Lodz (Poland)and the University of Antwerp (Belgium).In 2006 he was appointed as honorary member of the European Histamine Research Society.

For the period 1995 – 2005 he was listed as nr 55 on the list of worldwide top-100 most cited authors in the field of pharmacology and toxicology, being the highest in the Netherlands.

PL - 03

Plenary Lectures

Medicinal chemistry, an ever evolving discipline

Henk Timmerman
VU University Amsterdam, Netherlands.

ABSTRACT

Medicinal chemistry may be defined as the art to design -and subsequently to synthesise and pharmacologically characterise- on basis of information on structure- property relationships new compounds which should have the right pharmacological and toxicological profile for being suitable as active ingredient in medicinal products.

For obvious reasons medicinal chemistry could only emerge when organic synthesis became possible; that was around 1855. Until than medicinal products were derived either from biological sources (mainly plants) or metal oxides or salts. The first class contained mainly inactive or only weakly active preparations, the second could be described as especially toxic products. When synthetic medicines were introduced scientists realized that the chemical properties should be seen as also responsible for their biological effects; structure- activity relationships were already in the 1880-ies studied! There was an early euphoria and some investigators expected that soon "medicines could be designed (!!) for any disease". That was before 1900.

Things developed in a much different way. It was organic chemistry which determined for a long period the progress in medicinal chemistry. Organic chemists synthesised new derivatives which were accessible and pharmacologists searched for useful properties by screening procedures in vivo. Finding new useful compounds was a matter of trial and error and especially luck. Around 1935 the famous pharmacologist Clark sighed that "we have studied structure-activity relationships so intensively that we have a fair knowledge about the extend of our ignorance". The reasons for the failures were manifold, but especially the absence of useful parameters for biological activities made it impossible to derive at useful insights into the relationships between chemical structure and biological property of organic molecules.

When in the 1960-ies pharmacology changed into in vitro methods and molecular pharmacology was introduced pharmacology (better pharmacological parameters) started to become responsible for progress in medicinal chemistry; so-called selective compounds became attractive. When somewhat later in time computers became available for complex calculations, a boost in the studies structure - activity relationships could be observed. QSAR became a trendy approach and again scientist predicted that it would become relatively easy to design new medicines.

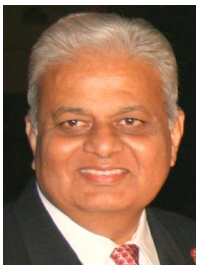
The results of applying the new methodologies were disappointing. The reason was a very intrinsic problem when trying to arrive at new medicines. A medicine cannot be described by one single property. Of course the an active ingredient of a medicine should have a certain property- such as a stimulatory or a blocking effect for a given receptor-, but it should also have certain pharmacokinetic properties, other activities should be absent (side effects) and the toxicity profile should at least guarantee a good therapeutic window. Currently it is more or less possible to design compounds having a predicted property, but that is not sufficient for making useful medicines.

During more recent years is has been the introduction of molecular biology, the advancement in analytical technologies, the emerging of systems biology, the availability of extremely powerful computers which determine the enormous progress in the possibility to derive at very interesting compounds, A major hurdle remains however the complexity of the profile of any compound for making it useful for medicinal applications. This truly intrinsic problem is a very tough one and one might therefore have some doubts whether it will ever be possible to design a new medicine.

In this presentation historical aspects will be presented, together with a personal opinion about coming developments. An essential characteristic of medicinal chemistry will receive special attention; the field can only flourish an approach in which several disciplines are integrated. The meaning of this conclusion for teaching and training medicinal chemistry will be emphasized as well.

PL - 05

Plenary Lectures



Dr. Rashmi H. Barbhaiya

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Rashmi H. Barbhaiya, Ph.D. is a Pharmaceutical Executive with 30 years of experience in Pharmaceutical R&D. He has a unique blend of management experience in Drug Discovery, Development and Life Cycle Management. He is one of the founders, CEO and Managing Director of Advinus Therapeutics, a research-based pharma company located in Bangalore and Pune, India.

Dr. Barbhaiya started his industrial pharmaceutical career in 1980 with Bristol-Myers Company in United States where he spent the next 21 years. The diversity of his background and experience has played a key role in speedy and successful development of a number of drugs for the treatment of a variety of diseases such as, AIDS and other infectious diseases, cancer, depression, anxiety, hypertension, CHF, diabetes and mild to moderate pain, including migraine. In the capacity of Vice President in the Pharmaceutical Research Institute of Bristol-Myers Squibb, he also played a key role, working with the drug discovery organization, in introducing "developability" as a key criterion in lead optimization and selection of drug candidates. As a result, there was significant reduction in timelines for discovery to development transition and for completion of preclinical development for IND filings.

In the year 2002, he returned to India to join Ranbaxy as the President of R & D and led a team of over 900 professionals involved in drug delivery and innovation-driven new drug research and development activities. He is credited for attracting world-class experienced scientists from overseas and for enhancing an innovation-driven culture to create one of the leading pharmaceutical R & D organizations in India. He was instrumental in creating an R & D alliance between Ranbaxy and GSK, the first of its kind for an Indian company. He is also credited for creating an alliance between Medicine for Malaria Venture (MMV) and Ranbaxy for developing a novel antimalarial which is currently undergoing Phase III clinical trials.

He obtained the Ph.D. degree in Clinical Pharmacology from the St. Bartholomew's Hospital Medical College, University of London. He continued his education through post-doctoral training at the University of Florida and University of Wisconsin. His scientific contributions have resulted in over 150 publications. He has helped to organize a number of scientific symposiums around the world. He is a member of several professional societies, among them are AAPS, ASCPT and ISSX. He has served on the Editorial Boards of Antimicrobial Agents and Chemotherapy as well as Biopharmaceutics and Drug Disposition journals. Dr. Barbhaiya has received a number of awards for his scientific contributions. Some of these include AAPS Fellow, AAPS Meritorious Manuscript Award, AAiPS Outstanding Achievement Award, Ranbaxy Award for Excellence in Pharmaceutical Research and India Life Sciences Person of the Year 2007 by Burrill & Company.

PL - 05

Plenary Lectures

India providing a solution for Pharma R & D Productivity Issues: Beyond Cost Arbitrage and Other Common Considerations

Rashmi H. Barbhaiya, Advinus Therapeutics Ltd, A Tata Enterprise, Bangalore, India

Spiraling increases in Pharma R & D spending over the last few years have not produced parallel increase in productivity as judged by the introduction of new drugs. The widening gap between R & D spending and productivity is no longer sustainable. The industry has no choice but to look for alternate models. Countries from emerging markets may offer a solution for addressing R & D productivity. Cost arbitrage is an obvious advantage that a country like India will offer. The current climate for R & D in India may offer something above and beyond cost arbitrage.

Innovation by definition requires risk taking. There is general feeling that most large organizations are risk averse and decision making takes time due to involvement of multiple committees. This is where emerging Pharma R & D in developing countries may make a difference. Newly established and small companies in Asia do not have past legacies, biases based on past successes or failures and they do not have any choice but to take risk. In addition, decisions in these emerging companies are usually taken by a handful of senior management professionals; seldom involving multiple committees.

The presentation will cover a story on how Tata motors developed Nano car – a classic example of disruptive innovation. It will end with an example of how Advinus has approached drug discovery for a difficult diabetes target.

PL - 06

Plenary Lectures

Prof. Colin Suckling

Freeland Professor of Chemistry, WestCHEM, Department of Pure & Applied Chemistry, University of Strathclyde, Glasgow, G1 1XL, Scotland
E-mail: c.j.suckling@strath.ac.uk
URL://www.chem.strath.ac.uk/people/academic/colin_j_suckling

Colin Suckling has been Freeland Professor of Chemistry at the University of Strathclyde since 1989. During the 1990s until 2002, he served successively as Dean of the Faculty of Science, Deputy Principal, and Vice Principal of the University of Strathclyde. Much of Professor Suckling's work during that time was strategic including the development of inter-institutional and interdisciplinary research partnerships notably the research collaboration with the University of Glasgow (WestCHEM), which was recognized publicly with the award of OBE in 2006.

Recent and current research interests focus on the synthesis and properties of heterocyclic compounds designed as molecular probes for biological systems or as drugs. Particular progress has been made in the field of fused pyrimidine compounds with anticancer and antiparasite activity and in the field of minor groove binders for DNA with antibacterial activity. Several discoveries are entering preclinical development.

Professor Suckling's standing in the field of heterocyclic chemistry has been recognized by the award of the Adrien Albert Lectureship of the Royal Society of Chemistry (2009-10) and his appointment as chairman of the 2011 International Congress of Heterocyclic Chemistry to be held in Glasgow.

PL - 06

Plenary Lectures

Heterocyclic chemistry at the edge of biology and medicine – The past, present, and future of Wsg1060

Colin J. Suckling
WestCHEM, Department of Pure & Applied Chemistry, University of Strathclyde, Glasgow, Scotland

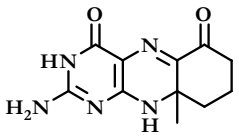
ABSTRACT

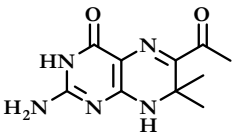
Wsg1060 is a member of a family of so-called blocked dihydropterins first synthesised at Strathclyde in the 1970s [*J. Chem. Soc., Perkin Trans. 1,* 1985, 1645] in a project initiated by the late Professor Hamish Wood aimed at the discovery of inhibitors of folate biosynthesis as potential antibacterial compounds. Apart from its unusual tricyclic structure, wsg1060 did not show any remarkable properties although its simpler bicyclic analogue, wsg1002, was shown to be synergistic with methotrexate in antibacterial assays. With one exception, a cyclopropane-containing irreversible inhibitor of dihydrofolate reductase [*J. Chem. Soc. Perkin Trans. 1,* 1992, 1299], the chemistry of this class of compounds lay dormant until the mid-2000s by which time it was well established that tetrahydrobiopterin BH_4 is the naturally occurring cofactor for several oxidation reactions including aromatic amino acid biosynthesis and nitric oxide synthesis. All of these reactions have been implicated in a number of pathologies.

The chemical instability of BH_4 contrasted strongly with the chemical stability of the blocked dihydropterins including wsg1002 and 1060. We wondered whether the blocked dihydropterins as a class might have a place as analogues of BH_4 in studies of nitric oxide synthases. In contrast to most medicinal chemical studies of enzymes as drug targets, we have been investigating the *activation* of nitric oxide synthases by analogues of BH_4 [*Bioorg. Med. Chem. Lett.* 2008, *18*, 1552–1555]. In collaboration with Professor Roger Wadsworth (Pharmacology, Strathclyde) we have shown that a number of blocked dihydropterins including both wsg 1002 are activators of iNOS in macrophages and eNOS in endothelial cells [*European J. Pharmacol.* 2010, DOI:10.1016/ j.ejphar.2010.09.070)]. This has led to proof of concept in vivo studies that suggest that blocked dihydropterins may have a role as drugs to treat cardiovascular disorders.

However, in order to understand better the structural properties that relate to NOS activation in this class of compounds and to seek compounds with potentially improved bioavailability, we have investigated the synthesis and properties of a range of blocked dihydropterins with substituent variations in both rings. Both target and diversity oriented syntheses have been developed and will be described. With a library of BH_4 related compounds available it is possible to begin to ask more detailed questions about the role of the pterin in proton and electron transfer in NOS. In collaboration with Dr Simon Daff (EastCHEM, Edinburgh) using the nNOS isoform we have found that wsg1060, as its tetrahydro derivative, is a highly competent substitute for BH_4 with very similar kinetic parameters.

Returning to the original reasons for making wsg1060, it has been re-evaluated in antibacterial assay in collaboration with Professor Andrew Hanson (Florida, USA) and found to be effective against *E. coli*. New leads against Gram negative bacteria are rare. Wsg1060 has thus become a key compound with potential to stimulate new drug discoveries in more than one important field.


wsg1060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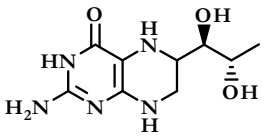

tetrahydrobiopterin

PL - 07

Plenary Lectures

Dr. Bharat K. Trivedi

CSO, Medicinal Chemistry, Drug Discovery, Wockhardt R & D, Aurangabad, India

EXPERIENCE (POSITIONS HELD)

June 2000 to Present: PGRD, Ann Arbor Laboratories, Pfizer Inc., Department of Medicinal Chemistry, 2800 Plymouth Road, Ann Arbor, Michigan, 48105.
October 1982 to June 2000: Parke-Davis Pharmaceutical Research, Division of Warner-Lambert Company, Department of Medicinal Chemistry Ann Arbor, Michigan, 48105.
March 2000 to Present: Director of Atherosclerosis Chemistry
I am currently responsible for directing atherosclerosis chemistry group, which includes 14 synthetic chemists. My primary responsibility includes supervision of senior synthetic chemists, and programs within the Atherosclerosis Team. The team is involved in developing number of strategies, which include both lipid targets and direct vessel-wall targets. I am currently a member of the Cardiovascular Discovery Team in Ann Arbor. The team is responsible for strategic review of the programs within the Cardiovascular Discovery Portfolio. As a member of the "Chemistry Senior Staff, I am involved in discussions regarding overall strategy for the chemistry department, including career development *I* promotions of colleagues. I am currently responsible for developing a program for "minority recruiting in chemistry", and I am the chair of the "Academic-Industrial Relations" committee.

PROFESSIONAL SOCIETIES AND ACTIVITIES

- Elected to Marquis "Who's Who in the Midwest" 23rd Edition (1992 to 1993).
- Recipient of the 2004 PGRD Achievement Award.
- Treasurer of the "Division of Medicinal Chemistry", American Chemical Society (January 2000 -Present)
- Interim Treasurer of the Division of Medicinal Chemistry, American Chemical Society (Jan 1999 -December 1999)
- Member of the "Executive Committee of the Division of Medicinal Chemistry", American Chemical Society, (January 1999 to Present).
- Member of the "Long-range Planning Committee, Division of Medicinal Chemistry", American Chemical Society, (January 1999 to Present).
- Member of the Award Selection Committee, American Chemical Society, 2002.
- Member of the Award Selection Committee, American Chemical Society, 2003.
- Member of the Award Selection Committee, American Chemical Society, 2004.
- Member of the Advisory Council to the Dean of College of Engineering and Science, University of Detroit (Fall 2002 to Present)
- "Secretary of the Medicinal Chemistry Section" of the Division of Chemistry and Human Health of IUPAC (January 2000 -January 2002)
- Member of the "International Advisory Committee" of the AFMC sponsored AIMECS Symposium 2003 in Kyoto, Japan
- Member of the International Advisory Board of the AFMC sponsored symposium on "Drug Discovery and Development in the 21st Century" which was held in the IUPAC Congress Meeting in Brisbane, Australia, 2001.

PL - 07

Plenary Lectures

Will India ever produce the first indigenous new drug for global market ?

Dr. Bharat K Trivedi
CSO, Medicinal Chemistry, Drug Discovery, Wockhardt R & D, Aurangabad, India

ABSTRACT

Of late, there has been a lot of debate and discussion, particularly in the print media, as to where we stand in terms of introducing innovative drug from India. The Pharma Industry has been practicing the art & science of "Drug Discovery & Innovation" for the past 15 years or more. Yet, the attainment of an ultimate goal - "introduce a product on the market" remains some what distal & illusive! The question is, are we even closer to reality? Do we have the appropriate leadership, know-how, experience and skill sets to develop thorough understanding of issues and challenges associated with both pre-clinical (discovery) & clinical (development) strategies to discover differentiable novel therapy? Have we considered factors such as "doability & drugability" of a given target both from bio- and chemo-centric perspectives? What have we learned from the so-called "early failures", and have we accordingly taken prudent measures to succeed in the future? This talk will attempt to address some of these questions, and provide "food for thought" as to what will it take to ultimately "get there" – i.e. "Introduce an innovative drug on the market"!

PL - 09

Plenary Lectures

Dr. Mukund S. Chorghade

President & Chief Scientific Officer, THINQ Pharma, 14 Carlson Circle, Natick, MA 01760-4205 USA
Tel: 1-508-651-7809, Mobile: 1-508-308-3891, Fax: 1-508-651-7920
E-mail: Chorghade@comcast.net

Dr. Mukund Chorghade is President of Chorghade Enterprises and Chief Scientific Officer, THINQ Pharma. He provides consultations to pharmaceutical researchers on collaborations with academic, government and industrial laboratories. He advises technology based companies on process re-engineering and project management of technology transfer; establishes strategic partnerships and conducts cGLP/cGMP compliance training and implementation in chemical laboratories. He oversees projects in medicinal chemistry, chemical route selection, process development, manufacturing and formulation of bulk actives to finished dosage forms.

Dr. Chorghade earned his B. Sc. and M. Sc. degrees from the University of Poona in India and a Ph. D. in organic chemistry at Georgetown University in Washington, D. C.. He completed postdoctoral appointments at the University of Virginia and Harvard University, visiting scientist appointments at University of British Columbia, College de France / Universite' Louis Pasteur, Cambridge and Caltech and directed research groups at Dow Chemicals, Abbott Laboratories, CytoMed and Genzyme. A recipient of three "Scientist of the Year Awards", he is an elected Fellow of the ACS, AAAS and RSC and has been a featured speaker in several national and international symposia. He is active in ACS, was NESACS and Brazosport Chair and serves on the International Activities Committee.

PL - 09

Plenary Lectures

Reverse pharmacology and systems approaches for chemical biology, drug discovery and development: Inspiration from mother nature and the wisdom of the Rishis

Mukund S. Chorghade*
THINQ Pharma, 14 Carlson Circle, Natick, MA 01760-4205 USA
E-mail: Chorghade@comcast.net

ABSTRACT

While biotechnological advances, genomics and high throughput screenings or combinatorial and asymmetric syntheses have long promised new vistas in drug discovery, the pharmaceutical industry is facing a serious innovation deficit. Critics suggest that "we have become high throughput in technology, yet have remained low throughput in thinking". Post marketing failures of blockbuster drugs have become major concerns of industries, leading to a significant shift in favor of single to multi targeted drugs and affording greater respect to traditional knowledge. Typical reductionist approach of modern science is being revisited over the background of systems biology and holistic approaches of traditional practices. Scientifically validated and technologically standardized botanical products may be explored on a fast track using innovative approaches like reverse pharmacology and systems biology, which are based on traditional medicine knowledge. Traditional medicine constitutes an evolutionary process as communities and individuals continue to discover practices transforming techniques. Many modern drugs have origin in ethnopharmacology and traditional medicine. Traditions are dynamic and not static entities of unchanging knowledge. In many parts 'little traditions' of indigenous systems of medicine are disappearing, yet their role in bioprospecting medicines or poisons remains of pivotal importance. Indian Ayurvedic and traditional Chinese systems are living 'great traditions'. Ayurvedic knowledge and experiential database can provide new functional leads to reduce time, money and toxicity - the three main hurdles in the drug development. We begin the search based on Ayurvedic medicine research, clinical experiences, observations or available data on actual use in patients as a starting point. We use principles of systems biology where holistic yet rational analysis is done to address multiple therapeutic requirements. Since safety of the materials is already established from traditional use track record, we undertake pharmaceutical development, safety validation and pharmacodynamic studies in parallel to controlled clinical studies. Thus, drug discovery based on Ayurveda follows a 'Reverse Pharmacology' path from Clinics to Laboratories. Herein we describe such approaches with selected examples based on previous studies.

We have launched a company-"THINQ Discovery" to derive inspiration and intellectual value from the wisdom of the Rishis to discover and develop New Chemical Entities for a variety of pharmaceutical, agrochemical and cosmoceutical applications. Traditional Medicine (Complimentary Alternate Medicine to the Western World) has historically involved clinical use of extracts, powders and other formulations. The extracts have not been standardized, the pure chemical products have rarely been isolated, the biological mechanisms of action have not been elucidated and the clinical trials have rarely been controlled and documented to international standards. THINQ's goals are to discover and develop these medicines to international standards and introduce them globally after appropriate regulatory filings.

PL - 10

Plenary Lectures

Prof. Ulrich Jordis

Institute of Applied Synthetic Chemistry, University of Technology,
Getreidemarkt 9, 1060 Vienna, Austria
E-mail: ulrich.jordis@tuwien.ac.at

Education

Vienna University of Technology
Diploma Thesis 1972 (academic title "Dipl.-Ing.")
Ph.D. in Organic Chemistry with Prof. F. Sauter (1974) Thesis: "Synthesis of novel pyrazol derivatives via 1,3-dipolar cycloadditions"
"Habilitation" (=lecturing qualification) 1989 , entitled to "Univ. Doz."

Professional Appointments

1973-1974	Inst. Organic Chemistry, Vienna, Teaching/Research Assistant
September 1975- August 1976	Massachusetts Institute of Technology (M.I.T.) Fulbright Research Fellow (Post-Doc with Sidney M. Hecht: synthesis of the bithiazole-part of bleomycin, pyrazolo[3,4-e]pyrimidines)
1983 (June - September)	University of Illinois at Urbana IL, Fulbright Research Associate with Prof. Nelson J. Leonard
1976-1989	(with 4 months sabbatical in 1983) Vienna University of Technology, Research Assistant
since 1989	Vienna University of Technology, Associate Professor

Other professional activities

- Head of the working-group "Computers in Chemistry" of the Austrian Chemical Society (1994-2002)
- Austrian Coordinator of COST D 16 Action (Combinatorial Chemistry) (since 1999)

Current research interests

Synthesis of Galanthamine-type natural products and analogs, combinatorial chemistry and solid phase synthesis, chemistry databases, modified nucleosides as potential antivirals, triterpene natural product analogs as hydroxysteroid dehydrogenase inhibitors, bridged piperazines as building blocks for the pharmaceutical industry, HPLC analysis of drugs and drug metabolites, synthesis of drug metabolites and labeled analogs, GC-MS analysis of prehistorical wood tar pitches including samples from the Tyrolian ice-man.

Expert in Chemistry Databases

PL - 10

Plenary Lectures

Synthesis and SAR of new glycyrrhetinic acid derived derivatives as 11β-hydroxysteroid dehydrogenase inhibitors

Ulrich Jordis[a] Laszlo Czollner[a], Christian Stanetty[b], Alex Odermatt[c], Paul Kosma[b], Dirk Claßen-Houben[d]

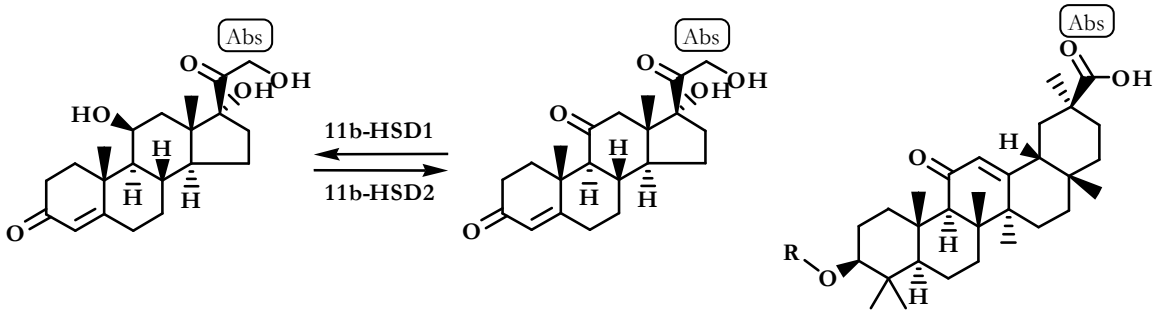
[a]Institute of Applied Synthetic Chemistry, University of Technology, Getreidemarkt 9, 1060 Vienna, Austria; [b]Department of Chemistry, University of Natural Resources and Applied Life Sciences, Muthgasse 18, 1190 Vienna, Austria; [c]Division of Molecular and Systems Toxicology, Pharmacenter, University of Basel, Klingelbergstrasse 50, 4056 Basel, Switzerland; [d]Onepharm Research and Development GmbH, Veterinärplatz 1, 1210 Vienna, Austria

E-mail: ulrich.jordis@tuwien.ac.at

ABSTRACT

Glycyrrhetinic acid, the metabolite of the natural product glycyrrhizin, is a well known nonselective inhibitor of 11β-hydroxysteroid dehydrogenase (11β-HSD) type 1 and type 2. Whereas inhibition of 11β-HSD1 is currently under consideration for treatment of metabolic diseases, such as obesity and diabetes, 11β-HSD2 inhibitors may find therapeutic applications in chronic inflammatory diseases and certain forms of cancer.

The talk will outline the background of the inhibition of 11β-HSD and summarize synthesis and SAR of novel glycyrrhetinic acid derivatives and analogs.



cortisol — cortisone — lycyrrhetinic acid: R = H; carbenoxolone: R = succinyl

REFERENCES

[1] Stanetty, Christian; Czollner, Laszlo; Koller, Iris; Shah, Priti; Gaware, Rawindra; Da Cunha, Thierry; Odermatt, Alex; Jordis, Ulrich; Kosma, Paul; Classen-Houben, Dirk. *Bioorg. Med. Chem.* (2010), 18(21), 7522-7541.

[2] Classen-Houben, Dirk; Kueenburg, Bernhard; Kosma, Paul; Jordis, Ulrich; Stanetty, Christian; Czollner, Laszlo. N-hydroxy C29-amide derivatives of oleandrane for the treatment of diseases mediated by 11beta-HSD WO 2010103046 (2010).

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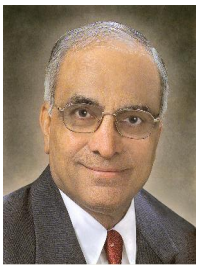
Plenary Lectures



Dr. Mulchand S. Patel

SUNY Distinguished Professor, UB Distinguished Professor, Associate Dean for Research & Biomedical Education, University at Buffalo (UB), The State University of New York (SUNY), Department of Biochemistry, School of Medicine and Biomedical Sciences 140 Farber hall, 3435 Main Street, Buffalo, NY 14214 USA
Tel: (716)829-3074; Fax: (716)829-2725; Email: mspatel@buffalo.edu

Education Bachground

B.Sc. (Chemistry), 1961, M. G. Science College, Gujarat University
M.Sc. (Biochemistry), 1964, M.S. University of Baroda
Ph.D. (Animal Scence), 1968, University of Illinois, Urbana-Champaign, USA

Research Experience

Assistant Professor of Research Pediat/Med., Temple University, Jan. 1970-June '75
Research Assistant Professor of Biochemistry, Temple University, Jan. 1970-June '75
Research Associate Professor of Biochem. & Med., Temple Univ., July 1975-June '78
Associate Professor of Biochemistry, Case Western Reserve Univ., July 1978-June '86
Professor of Biochemistry, Case Western Reserve University, July 1986-April '93
Chairman, Dept. of Biochemistry, SUNY at Buffalo, 1993-'98

Publications: 225

Books edited: 6

Awards

Vice-Chancellor C.S. Patel Gold Medal in Biochem.,1972-73, M.S.Univ. ofBaroda
Fulbright Research Scholar Award,1987, M. S.University of Baroda
The Stockton Kimball Award-2004, Sch. Med. Biomed. Sci., Univ. at Buffalo, 2004
Research &Scholarship Award, Research Foundation, SUNY, 2007

Memberships in Scientific Committees and Journals

NIH, Biochemistry Study Section 2, July 1984 -June 1988
NIH/NIDDK Special Grant Review Committee, Subcommittee B, July 1991-June '95
Editorial Board, *American Journal of Physiology*, July 1988 - June 1994
The Biochemical Journal, Editorial Adviser, 1991-1998
Editorial Board, *The Journal of Biological Chemistry*,'91-97;'99-2004;'06-present
Editorial Board, Metabolic Syndrome and Related Disorders, 2003-present
Editorial Board, Current Trends in Biotechnology and Pharmacy, 2008-present
American Society for Biochemistry and Molecular Biology, 1974-present
American Society for Nutritional Sciences, 1971-present

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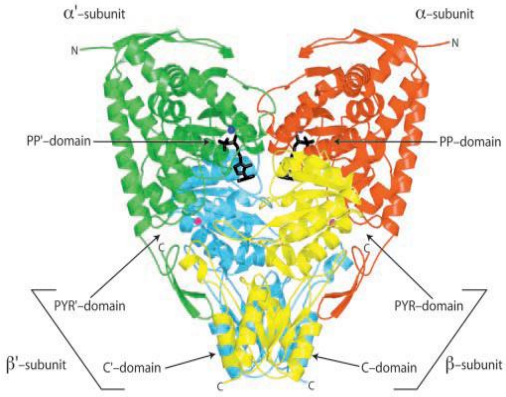
Plenary Lectures

Human pyruvate dehydrogenase complex: Structure-function relationship and regulation

Mulchand S. Patel
Department of Biochemistry, School of Medicine and Biomedical Sciences, University at Buffalo, The State University of New York, Buffalo, NY, 14214 USA
E-mail: mspatel@buffalo.edu

ABSTRACT

The human (h) pyruvate dehydrogenase (PDH) complex (PDC) is composed of multiple copies of three catalytic components (PDH, E2, and E3), E3-binding protein (BP) and regulatory PDH kinases (PDKs) and phosphatases [1, 2]. The presence of BP in PDCs from higher eukaryotes is unique for its integration in the central E2/BP core and also for binding of E3 [3]. hPDH, a thiamin pyrophosphate-requiring enzyme with an α2β2 structure, catalyzes first two successive steps in PDC catalysis: the decarboxylation of pyruvate to CO_2 and the reductive acetylation of the lipoyl groups of hE2. hPDH has two active sites at the interface of two subunits (see figure). Based on crystal structure of hPDH it is suggested to function by a flip-flop mechanism through a concerted ~2Å shuttle-like motion of its heterodimers [4]. Catalytic events are predicted to cause movements transmitted from one active site to the other through a triad of residues and the interdomain interactions. Regulation of hPDC activity is accomplished by a family of PDKs and phosphatases [1]. Three serine residues (sites 1-3) in the α subunit of hPDH are phosphorylated. hPDH displays half-of-the-site reactivity during phosphorylation as phosphorylation of a single site is sufficient for hPDH inactivation [5]. Regulation of hPDC activity by 4 PDK isoenzymes with different site-specificity and tissue distribution plays a critical role in type 2 diabetes and in some forms of cancers (the Warburg effect). Hence inhibition of PDKs by small molecule inhibitors is of interest for these disease states.



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Plenary Lectures

Prof. Michael D. Threadgill

Department of Pharmacy & Pharmacology, University of Bath, Claverton Down, Bath BA2 7AY
Tel: +44 1225 386840; Mobile: +44 7867 805919; Fax: +44 1225 386114
E-mail: m.d.threadgill@bath.ac.uk

Qualifications

1998	DSc	University of Bath
1981	PhD	Organic Chemistry, University of Cambridge *Supervisor*: Professor Sir Alan Battersby FRS *Thesis*: Synthetic studies related to cytochrome oxidase
1978	M A	University of Cambridge
1975	PGCE	University of Durham
1974	BA	Natural Sciences Tripos, University of Cambridge *Part 1a*: Chemistry, Cell Biology, Physics, Mathematics *Part 1b*: Chemistry, Biochemistry *Part 2*: Chemistry

Employment

November 2008 – present	Professor in Medicinal Chemistry Head of Medicinal Chemistry Department of Pharmacy & Pharmacology, University of Bath
March 2000 – October 2008	Reader in Medicinal ChemistryDepartment of Pharmacy & Pharmacology, University of Bath
September 1993 – February 2000	Senior Lecturer in Medicinal ChemistryDepartment of Pharmacy & Pharmacology, University of Bath

Current research interests and group

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

Inhibition of PARPs: one PhD student (funded by KuDOS Pharmaceuticals and University of Bath)
Inhibition of Tankyrases: One postdoctoral researcher and two PhD students (funded by AICR and University of Bath)
Inhibition of DHFR of M. tuberculosis: One PhD student (funded by Saudi Government)
Polymeric prodrugs: One PhD student (funded by Prostate Cancer Charity).

Current teaching

My teaching is mainly of medicinal and biological chemistry, with some spectroscopy. My contact hours are *ca.* 140 hours per annum and I convene the major introductory chemistry module for first-year students of Pharmacy and of Pharmacology.

PL - 12

Plenary Lectures

Isoform-selective inhibitors of PARP-2: Design, synthesis and evaluation

Michael D. Threadgill,[a] Peter T. Sunderland,[a] Mary F. Mahon,[a] Niall M. B. Martin,[b] Pauline J. Wood[a] and Esther C. Y. Woon[a]

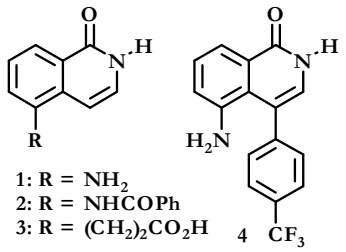
[a]Medicinal Chemistry, Department of Pharmacy & Pharmacology, University of Bath, Bath BA2 7AY, UK. [b]KuDOS Pharmaceuticals Ltd, 410 Cambridge Science Park, Cambridge CB4 0PE, UK.

ABSTRACT

PARP-2 is a poly(ADP-ribose) polymerase, with some activities similar to those of PARP-1 but with other distinct roles.[1] Non-isoform-selective inhibitors are in clinical trial for the treatment of cancer.[2] Isoform-selective inhibitors would enable studies on the specific roles of PARP-2 in the mammalian cell. Three series of isoquinolin-1-ones were designed as selective inhibitors of PARP-2, using the X-ray structures of the isoforms.

For the first series, 5-aminoisoquinolin-1-one (5-AIQ, **1**, a potent non-isoform-selective inhibitor),[3,4] was acylated with a diverse series of aromatic and bulky aliphatic acid chlorides to give 5-benzamido- and 5-acylamino-isoquinolin-1-ones. A new route to 5-AIQ has been devised (nitration of 1-chloro-isoquinoline, hydrolysis of 1-chloro-5-nitroisoquinoline and hydrogenation) which provides this important agent in high yield without chromatography. The second series comprised isoquinolin-1-ones carrying carboxylic acids tethered to the 5-position, designed to bind to a Lys side-chain in the PARP-2 structure. For example, Heck coupling of 5-iodoisoquinolin-1-one with propenoic acid, followed by hydrogenation, gave **3**. The third series comprised 4-substituted 5-AIQ derivatives. These were prepared by Pd-catalysed couplings to 1-alkoxy-4-bromo-5-nitroisoquinolines, which proceeded efficiently, even with very bulky arylboronic acids as Suzuki coupling partners. Twenty-eight isoquinolin-1-ones were evaluated *in vitro* for inhibition of the PARP-1 and PARP-2 isoforms. The most selective PARP-2 inhibitors were **2** (9.3×) and **4** (7.6×) and showed greater selectivity than a reported lead (5-benzoyloxyisoquinolin-1-one)[5] in a comparative study. None of the compounds were strongly cytotoxic towards four human tumour cell lines (HT29 colon carcinoma, MDA-MB-231 breast carcinoma, LNCaP prostate carconima, MOLT4 T-cell leukaemia) and one normal cell line (FEK4 fibroblast).

The most isoform-selective compounds will be used in ongoing studies of the intracellular role(s) of PARP-2.



1: R = NH_2
2: R = NHCOPh
3: R = $(CH_2)_2CO_2H$
4

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Plenary Lectures

Prof. Domenico Spinelli

Dipartimento di Chimica 'G. Ciamician', Alma Mater Studiorum, Bologna (Italia)
E-mail: domenico.spinelli@unibo.it

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.

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 - 13

Plenary Lectures

From 6-aryl-5-nitrosoimidazo[2,1-*b*][1,3]thiazoles to 8-aryl-8-hydroxy-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-ones: A new class of compounds showing a variegate reactivity and an interesting biological profile

Barbara Cosimelli[1] and Domenico Spinelli[2]
[1]Dipartimento di Chimica Farmaceutica e Tossicologica, Università degli Studi di Napoli 'Federico II' (Italia)
[2]Dipartimento di Chimica 'G. Ciamician', Alma Mater Studiorum, Bologna (Italia)
E-mail: domenico.spinelli@unibo.it

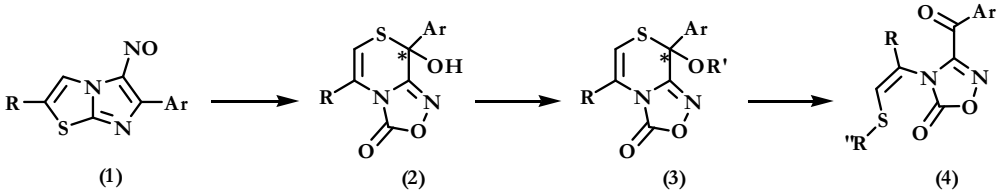
ABSTRACT

In the lecture a series of new reactions involving nitrosoimidazoles condensed with five- (1) or six-membered (2) rings will be described. Thus, 6-aryl-5-nitrosoimidazo[2,1-*b*][1,3]thiazoles 1 by treatment with hydrochloric acid provided *via* a ring-opening/ring-closing sequence the relevant 8-aryl-8-hydroxy-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-ones 2 (1), a new class of compounds with interesting chemical reactivity and biological profile.

As a matter of fact compounds 2, which contain a hemithioacetal cyclic structure, can react with alcohols in the presence of *p*-toluensulfonic acid giving the corresponding thioacetals, 8-aryl-8-alkoxy-8*H*-[1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-3-ones 3 (3), or with silver nitrate and reactive organic halide (haloalkanes, allylic and benzyl halides, and so on) furnishing the relevant 3-aryl-4[(*Z*)-1-methyl-2(alkylsulphanyl)-vinyl]-[1,2,4]oxadiazol-5(4H)-ones 4 (4).

Compounds 2 (5), 3 (3), and 4 (4) show interesting pharmacological activities: several of them showed a significant activity as L-type Ca^{2+} channel blockers (LTCCBs), some time more potent than diltiazem. The role of the substituents in the aryl moiety (3–5) and that of the chain in the acetal (5) as well as in alkylsulphanyl (4) groups have been evaluated and a virtual receptor scheme was derived for the binding site. Starting from this 3D QSAR model, virtual screening procedures were performed with the aim of identifying novel chemotypes for LTCCBs, starting from databases of purchasable compounds (6–7).

Moreover by examining the behavior of some 2 and 3 we have identified (8) some compounds able to contrast the phenomenon of multidrug resistance.



Scheme 1

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Plenary Lectures

Prof. Gree René

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Qualifications

pHD Thesis, University of Rennes (advisor: Prof. R. Carrié, 1975)
post-doctoral, Ohio State University Columbus (advisor: Prof. L.A. Paquette, 1977)

Present Position

Directeur de Recherches CNRS (equivalent to full Professor)
Codirector of the Indo-French "*Joint Laboratory for Sustainable Chemistry at Interfaces*" (LIA CNRS-UR1/IICT-CSIR India, 2008-2011)

Awards and Honours

Organic Chemistry Division Award of the French Chemical Society (1985)
Elected Maître de Conférences (Part time Lecturer), Ecole Polytechnique, Paris (1990-2002)

Present Research Interests

Organometallic chemistry and catalysis directed towards organic synthesis
Fluorine Chemistry
Medicinal chemistry (cancer, diabetes, CNS)
Chemistry in, and with, Ionic liquids

Scientific results

over 200 publications in scientific journals
Supervision of 50 phD thesis and 20 postdocs
Over 200 invited seminars and lectures, in France and many foreign countries including over 40 plenary lectures in international congress

Scientific Commitees

French representative for the COST D2 Action (selective synthesis) at the European Community, Brussels (1972-77)
Elected member of the CNRS committee for Organic Chemistry (1992-95)
President of the CNRS committee for Organic Chemistry (1995-2000)

Editorial Boards

6 international journals

Consultantship

Laboratoires Servier; Aventis; Evolva; Sapala; Chemveda

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Plenary Lectures

Total synthesis of bioactive natural products and designed structural analogues

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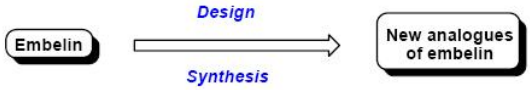
ABSTRACT

Natural products play important and multiple roles in chemistry, as well as in life sciences. They are not only challenging targets for total synthesis but they are also very useful starting material for enantioselective synthesis. On the other hand, they are highly valuable tools in bioorganic chemistry, in medicinal chemistry and in pharmacology.

During this lecture we will describe two examples of our research in this field:

- In the first part, we will report our results dealing with a new transition metal-catalyzed interconversion of sugars into functionalized and chiral carbocycles. Corresponding cycloalkenones are very useful intermediates in the synthesis of various types of bioactive molecules.[1] This new transposition has been extended to amino acid derived molecules, affording novel azasugar derivatives. Furthermore we have successfully developed new similar tandem isomerization-Mannich reactions which afford, in high ee's, natural products such as Nikkomycins and Funebrine, as well as new aminocyclitol compounds.

- In the second part we will describe the design, synthesis and preliminary data on biological evaluation of new analogues of embelin. This benzoquinone-type natural product has been reported to possess a large variety of biological activities such as anthelminthic, antifertility, antiimplantation, antibacterial and recently anticancer activity. Later property appears to be linked to induction of apoptosis for cancer cells, through inhibition of XIAP protein.[2] We will report on our research towards the preparation of new bioactive analogues of this natural product.[3]



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Plenary Lectures

Prof. Lutz Ackermann

Institute for Organic and Biomolecular Chemistry, Georg-August-University Göttingen, Tammannstrasse 2, 37077 Göttingen, Germany
E-mail: Lutz.Ackermann@chemie.uni-goettingen.de

Education and Research Experience

since 2007	Full Professor (W3) at the Georg-August-Universität Göttingen
2003 – 2007	Emmy Noether-Fellow (DFG) at the Ludwig-Maximilians-Universität München
2001 – 2003	Postdoctoral Studies with Prof. Dr. R. G. Bergman, UC Berkeley.
2001	PhD Universität Dortmund (*summa cum laude*)
1999	Research stay with Prof. Dr. P. H. Dixneuf at the Université de Rennes, France
1998 – 2001	PhD thesis with Prof. Dr. A. Fuerstner, Max-Planck-Institut für Kohlenforschung in Mülheim/Ruhr
1997 – 1998	Diploma thesis (MSc) with Prof. Dr. J. Mattay
1993 – 1998	Studies of Chemistry at the Christian-Albrechts-Universität zu Kiel

Awards and Distinctions

2010	Alphora Lecturer, University of Toronto
2009	Japan Society for the Promotion of Science (JSPS) Visiting Professor Fellowship
2008	Goering Visiting Professor, University of Wisconsin-Madison, USA
2007	Visiting Professor at the Università degli Studi di Milano, Italia
2007	Dozentenstipendium (Fonds der Chemischen Industrie)
2007	ADUC-price 2006
2006	Award of the Dr. Otto-Röhm-Gedächtnisstiftung
2006	Römer-fellowship 2006
2006	DuPont Center for Collaborative Research & Education Grant
2006	ORCHEM-Preis für Naturwissenschaftler
2006	G.I.F. Young Scientists' Program
2004	Thieme Journal Award
2003 – 2007	Emmy Noether-Programm, DFG
2001 – 2002	Postdoctoral Scholarship (DAAD)
1999 – 1999	Research Scholarship of the DAAD
1999 – 2001	Kekulé-fellowship (Fonds der Chemischen Industrie)
1998 – 1999	PhD Fellowship of the Max-Planck-Gesellschaft
since 2009	Member of the Editorial Advisory Boards of *Synlett* and of *Synthesis*

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Plenary Lectures

Metal-catalyzed C–H bond functionalizations for sustainable synthesis

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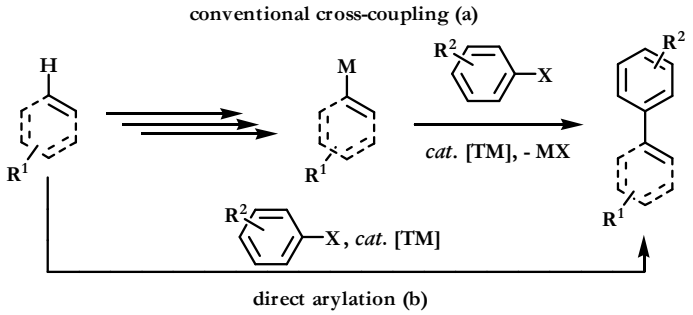
ABSTRACT

Metal-catalyzed cross-coupling reactions between organic (pseudo)halides and organometallic reagents are am ong the most important tools for C(sp^2)–C(sp^2) bond formations (*a*). The corresponding organometallic nucleophilic starting materials are, however, often not commercially available, and lead to the formation of side-products. Therefore, focus has shifted in recent years to catalytic direct arylations through C–H bond cleavages as economically attractive alternatives (*b*).[1]

The use of ruthenium, palladium or copper catalysts for efficient direct arylations of (hetero)arenes will be presented. Particularly, the development of generally applicable C–H bond functionalizations with aryl tosylates,[2a-c] and mesylates[2c] as well as unactivated alkyl halides bearing β-hydrogens[3] as inexpensive electrophilic substrates will be discussed.



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[3] **(a)** L. Ackermann, Chem. Commun. 2010, 46, 4866. **(b)** L Ackermann, P Novák, R Vicente and N Hofmann, Angew. Chem. Int. Ed. 2009, 48, 6045.

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Plenary Lectures

Prof. Ronald P. Jordan

Dean
College of Pharmacy, The University of Rhode Island, U.S.A.

Ronald P. Jordan is a registered pharmacist and Fellow of the American Pharmacists Association. He is in his 4th year as Dean of The University of Rhode Island, College of Pharmacy. Ron is an entrepreneur and pharmacy leader with business development and health informatics expertise. He founded businesses in hospice and pain management pharmacy, health benefit management software and integrated health systems informatics consulting. He was also a senior executive at companies offering an internet consumer prescription marketplace, pharmaceutical product supply chain transformation and health benefit insurance for 10 years. He earned his BS Pharmacy at URI and studied three years in a Doctoral program in pharmaceutics.

Ron is a former President of the American Pharmacists Association (APhA), the largest professional society of pharmacists in the world. Recently he was selected as a Dean Mentor for the American Association of Colleges of Pharmacy, Academic Leadership Fellows Program. He has also served a Trustee and Standardization Chairman of the National Council for Prescription Drug Programs (NCPDP), which develops consensus standards for the prescription drug benefit industry. As a volunteer leader at APhA, he was instrumental in moving community pharmacy toward a patient care focus and medication therapy management as a practice. He also led NCPDP in developing American National Standards Institute approved operating procedures used to create consensus standards for pharmacy and integrated electronic health records information. Both efforts were critical foundations for the long sought Medicare Part D prescription drug benefit.

Ron was one of eleven voting members, including two pharmacists, of the Health Care Financing Administration's Medicare Coverage Advisory Committee Panel on "Prescription Drugs, Biologicals and Therapeutics." The panel supplied advice and recommendations on national coverage policy under Medicare between 1999 and 2005. In 1998 and 1999 Mr. Jordan testified on electronic standards, security and administrative simplification at the Health and Human Services, National Committee on Vital Health Statistics, charged with investigating these areas and recommending actions to the Secretary under the Health Insurance Portability and Accountability Act (HIPAA) of 1996. Mr. Jordan was appointed by Rhode Island Governor Lincoln Almond to the Governor's Advisory Council on Health (GACH) and served from 1997-2003. He was Chairman of the GACH subcommittee on Prescription Drugs. In 1989, Ron was appointed to the HCFA Office of Research and Demonstration Advisory Panel developing the design for OBRA 1990 Federal Medicaid program demonstration projects on the cost effectiveness of online prospective drug utilization review and pharmacist reimbursement for cognitive services. Other notable government appointments include his work on development and implementation of the Rhode Island Pharmaceutical Assistance to the Elderly (RIPAE) Program with state legislative leaders in the mid 1980's. The program operated for years as one of the most cost efficient state elderly drug assistance programs. Ron has served previously on the Secretary of Health and Human Resources, WEDI (Workgroup on Electronic Data Interchange) Board of Directors and as an active member and subcommittee chair on the American National Standards Institute, Health Informatics Standards Planning Panel, and the Health Informatics Standards Board (HISB). He has also served as the US and Pan American Delegate to the Health Care work group of the United Nations EDIFACT international electronic data interchange standards group.

Mr. Jordan was twice cited as one of the 50 most influential pharmacists in the United States by *American Druggist*. He received the Rhode Island Pharmacists Association award for Innovative Pharmacy Practice twice and has received numerous other awards and professional recognition including the Kappa Psi Pharmaceutical Fraternity, Richard A Bliss, Grand Council Citation and Award for inspiring leadership and appreciation for unselfish service to Pharmacy and Pharmacy Education and the URI College of Pharmacy, Dr. Norman A Campbell Award for Ethics and Excellence in HealthCare both awarded in 2006. He has received numerous leadership awards and citations and has been made an Honorary Member of the New Jersey Pharmacists Association and the Pharmaceutical Society of Israel.

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Plenary Lectures

Single use biopharmaceutical production technology – Green, efficient and sustainable manufacturing

Ronald P. Jordan
Dean, College of Pharmacy, The University of Rhode Island, U.S.A.

ABSTRACT

This presentation will review the development and application of single use technology in the biopharmaceutical manufacturing space. This technology is a rapidly expanding approach that is showing strong performance in cell culture, filtration, purification and other process steps at both small and large scale. Innovators are delivering breakthroughs to the industry that eliminate or greatly reduce the need for intensive cleaning and steam sterilization steps and the equipment needed to perform them. This results in a modern, green manufacturing plant that is much more efficient, smaller, uses 70-80% less water, 30-50% less power and generates significantly reduced liquid waste streams. As the technology evolves further, other industries such as alternative energies, chemical processing, and agri-business will adapt these applications for their benefit.

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Plenary Lectures

Prof. Keykavous Parang

Professor of Medicinal Chemistry and Pharmacology, University of Rhode Island, Kingston, RI, 02881
E-mail: kparang@uri.edu

Positions and Employment

Oct. 2000-Present	Visiting Scholar, Johns Hopkins University School of Medicine, MD.
2001-2004	The Executive Editor of "Current Pharmaceutical Design".
2004-Present	Editorial Advisory Board "Current Medicinal Chemistry-Central Nervous System Agents".
2005-Present	Editorial Advisory Board of "Recent Patent Reviews on CNS Drug Discovery"
2007-Present	Editorial Board member of "Perspectives in Medicinal Chemistry"
2007-Present	Editorial Board Member of "Open Biochemistry Journal"
Dec. 2008-Present	Editorial Board Member of Associate Editors, "The Beilstein Journal of Organic Chemistry"
Oct. 2000-April 2008	Assistant and Associate Professor, Biomedical and Pharmaceutical Sciences, University of Rhode Island, RI.
April 2008-Present	Full Professor, Biomedical and Pharmaceutical Sciences, University of Rhode Island, RI.

Honors

- 1993-Mike Wolowyk Graduate Scholarship (University of Alberta)
- 1993-Myer Horowitz Graduate Scholarship (University of Alberta)
- 1994-Dr. Wu Hong Fund Poster Prize (University of Alberta, December 2, 1994)
- 1995-J. Gordon Graduate Student Award (University of Alberta, March 8, 1995)
- 1996-Golden Bulb Light Award (University of Alberta, March 1996)
- 1994-1996-Alberta Heritage Foundation for Medical Research Student Scholarship
- 1997-The Most Positive Influence Award (University of Alberta).
- 1997-Alberta Heritage Foundation for Medical Research Postdoctoral Fellowship
- 1998-American Chemical Society Travel Grant (Medicinal Chemistry Division) (Boston)
- 2001-Commercial Innovation Award, Slater Center For Biomedical Technology (University of Rhode Island)
- 2004-Outstanding Intellectual Property Development, University of Rhode Island
- 2009-Honarary Fellowship from Indian Society of Chemists and Biologists
- 2009- Harry and Elsa Jiler—American Cancer Society Professors Meeting Travel Scholarship
- 2010-Microbicide2010 Travel Scholarship

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Plenary Lectures

Peptide nanostructures as molecular transporters of therapeutic agents

Keykavous Parang
University of Rhode Island, Kingston, RI, 02881
E-mail: kparang@uri.edu

ABSTRACT

To date, most approaches that have been used for cellular delivery of compounds using peptides have taken advantage of covalent conjugation and/or endocytotic pathways. Endosomal entrapment represents a major challenge in targeted intracellular drug delivery. A number of amphipathic peptides were synthesized to create nanoscale self-assembled molecular transporters for the efficient non-covalent targeted delivery of therapeutics including anticancer agents. CD, transmission electron microscopy, and fluorescence spectroscopy were used to characterize and/or confirm the formation of the self-assembled structures. The peptides were designed systematically to non-covalently entrap or bind a hydrophobic drug and to enhance cellular delivery and active targeting. The data validated the effectiveness of this strategy using self-assembled peptides that exhibited encapsulation of camptothecin, higher cellular uptake of labeled lamivudine, and nuclear delivery of doxorubicin. The cellular uptake of labeled peptide was time dependent, rapid even after 5 min, and did not require endosome-derived vesicles. This is a key advantage to the endocytotic entry for known cell-penetrating peptides that require endosomal escape to passage the conjugate out of the resulting endosome. Taken together, the results will have significant implications for the design of more efficacious tools for delivery of hydrophobic and/or cell-impermeable compounds.

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Plenary Lectures

Prof. Ajayan Vinu

Senior Scientist, International Center for Materials Nanoarchitectonics, World Premier International Research Center, National Institute for Materials Science (NIMS), 1-1, Namiki, Tsukuba, Japan
E-mail: vinu.ajayan@nims.go.jp; apvinu@yahoo.com
http://www.nims.go.jp/super/HP/vinu/websitevinu/V-top.htm

Academic Highlights

2008 to till date: Senior Scientist of MANA and Research Director of NIMS-India Center
2006 to till date: Senior Researcher, Group Leader, NIMS, Japan
2004 to 2006: ICYS fellow, NIMS, Japan
2000 to 2003: PhD, Anna University, India (coll. with TUK, Kaiserslautern, Germany).
2001 to 2004: Research Associate, University of Kaiserslautern, Germany

Main Awards and Honors

Laureate of KIA for 2008, *Iran Top science award; Chemical Society of Japan Award for Young Chemists for 2008, Asian excellent young researcher lectureship award for 2008; Indian Society for Chemists and Biologists Award for Excellence 2010;* One of the Top 15 researchers in the world (mesoporous Materials) by "Science Watch"; Chairman of international conferences (10); PhD thesis examiner of Max Planck institute, University of Pune, Acharya University; Bhatnagar award (India highest science award) review committee member; Adjunct Principal Researcher of KRICT, Korea; Adjunct associate professor of Hokkaido University, Adjunct professor of Yonsei University, Korea.

Invited Lectures

More than 75 including several plenary lectures in various countries.

My present group

4 post docs; 4 PhD students; 2 research assistant, 2 visiting scientist (guided: 20 post docs; ca. 25 PhD students including the students who visited for a long period through the collaboration)

MOU signed with

10 universities around the world, RPI, KSU (USA), KRICT, Yonsei (Korea), ANU (Australia), NCL, JNCASR, AU, NIT (India) etc.

Research Achievements

Discoverer of Carbon Nanocage, mesoporous carbon nitride, carbon nitride nanocage molecular sieves, mesoporous BN and BCN materials, carbon nanocoops, and silica nanocoops, fullerenes and heteropolyacids.

Areas of Interest

Nanoporous Semiconductors, Nitrides, and carbons, Fuel Cells, Catalysis; Biocatalysis and biomolecule immobilization.

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Plenary Lectures

Fabrication and the applications of hierarchically ordered nano/ macroporous films and powders

Ajayan Vinu*
***International Center for Materials Nanoarchitectornics, World Premier International Research Center, NIMS, Tsukuba 305 0044, JAPAN.**
E-mail: vinu.ajayan@nims.go.jp

ABSTRACT

Carbon nitride (CN) is a well known and fascinating material that has attracted worldwide attention because the incorporation of nitrogen atoms in the carbon nanostructure can enhance the mechanical, conducting, field emission, and energy storage properties. CN materials with five different structures have been predicted so far: one is two dimensional graphitic C_3N_4 and four are three-dimensional carbon nitrides, namely α-C_3N_4, β-C_3N_4, cubic-C_3N_4, and pseudocubic-C_3N_4. Among the CN materials, β-C_3N_4 and its allotropic cubic and pseudo-cubic phases are superhard materials whose structure and properties are expected to be similar to those of diamond and β-Si_3N_4. Owing to its unique properties such as semi-conductivity, intercalation ability, hardness, CN is regarded as a promising material which could find potential applications in many fields. CN materials with no porous structure can be prepared either from molecular or chemical precursors at very high temperatures. By constructing CN materials with porous structure, many novel applications could emerge: from catalysis, to separation and adsorption of very bulky molecules, and to the fabrication of low dielectric devices. However, only a little attention has been given to the synthesis of porous CN materials.

Recently, we have introduced a new concept of making nanoporous carbon nitride materials via hard templating approach in which nanoporous silica was used as template.[1] In the first part of the talk, I will present some results about the discovery of the nanoporous carbon nitride materials, and the basics and the mechanism behind the synthesis of various nanoporous nitride materials with different pore structure and textural parameters. Then, the preparation, characterization and the applications of one and three dimensional nanoporous carbon nitrides materials synthesized using various inorganic templates with the different pore structures (MCN-1[1,2] and MCN-2[3]) through a simple polymerization reaction between ethylenediamine (EDA) and carbon tetrachloride (CTC) will be presented. Moreover, the methods to control the textural parameters and the nitrogen content of the nanoporous carbon nitride materials, especially with the nitrogen precursors with different nitrogen contents will also be discussed.[4,5] The fabrication of nanoporous carbon nitride nanoparticles with a size smaller than 50 nm which was prepared by using silica nanoparticles as templates, and films with hierarchical ordered nano/macroporous structure and morphology will also be demonstrated. One of the important features of the materials is that they have inbuilt basic sites in the form of NH_2 or NH groups and can be used as a metal free basic catalyst. These functional moieties on the surface of the nanoporous materials not only provide the basic sites for the catalytic reactions but can also be used as an adsorbent for the CO_2 molecules, stabilizer and reducing agent for the fabrication of the metal nanoparticles with ultra small size.[6] The basic catalytic efficiency of the materials in the synthesis of caprophenone (Figure 1), transesterification of beta-ketoesters with different alcohols, aldol and Knoevenagel reactions and their ability to capture acidic CO_2 molecules will also be demonstrated. In the second part of the talk, I briefly discuss about the different ways of preparing nanoporous carbon materials with various structure types, especially "Carbon Nanocage and Carbon Nanocoops", and to tune the pore diameters and textural parameters and the different ways of adding new functions on the surface of the nanoporous carbon materials. Moreover, the functions of the nanoporous materials in various fields such as sacrificial template,[7] adsorption and separation,[8] fuel cells, sensing,[9,10] catalysis, and magnetism[11] will be demonstrated.

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Plenary Lectures

Prof. Erik Van der Eycken

Laboratory for Organic & Microwave-Assisted Chemistry (LOMAC), Katholieke Universiteit Leuven (K.U.Leuven), Celestijnenlaan 200F, B-3001, Leuven, Belgium
Tel: +32/16/327406; Fax: +32/16/327990
E-mail: erik.vandereycken@chem.kuleuven.be

Erik Van der Eycken is Professor Organic Chemistry and head of the Laboratory for Organic & Microwave-Assisted Chemistry (LOMAC) at the University of Leuven (K.U.Leuven), Belgium. He received his Master diploma (1982) and his PhD degree (1987) in organic chemistry from the University of Ghent, Belgium, with Prof. Maurits Vandewalle on the total synthesis and structural elucidation of Specionin, an iridoid insect antifeedant. From 1988 to 1992 he worked as a scientific researcher at the R&D-laboratories of AGFA-Gevaert, Mortsel, Belgium. He moved back to the University of Ghent as a scientific collaborator on photo-induced reactions with Prof. Denis De Keukeleire and Prof. Piet Herdewijn on HIV-active drugs (1992-1995). From 1995-1997 he was connected to the Flemish Inter-University Institute for Biotechnology (VIB), Ghent, with Prof. Marc Van Montagu where he was involved in the synthesis of intermediates for the elucidation of biological reaction pathways. In 1997 he became Doctor-Assistent at the K.U.Leuven, Belgium in the group of Prof. Georges Hoornaert, where he was involved in heterocyclic chemistry. He was appointed part-time professor in 2004 at the same university and started his independent academic career. After short periods of postdoctoral work at the University of Graz (2002) with Prof. C. O. Kappe on microwave-assisted hetero-Diels-Alder reactions, at The Scripps Research Institute (La Jolla, USA) (2003) in the group of K. B. Sharpless, on microwave-asssisted click chemistry, and at Uppsala University (2004) with Prof. M. Larhed and Prof. A. Hallberg on microwave-assisted carbonylations, he was appointed full-time professor in 2007 at the K.U.Leuven. The main focus of his research is the investigation of the application of microwave irradiation in different domains of organic synthesis, i.e. synthesis of bioactive natural product analogues and heterocyclic molecules applying transition metal catalyzed reactions and solid phase organic synthesis. His lab is also active in the field of microwave-assisted synthesis of (cyclic) peptides and peptidomimetics.

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Plenary Lectures

Exploring the benefits of microwave irradition in heterocyclic chemistry

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Laboratory for Organic & Microwave-Assisted Chemistry (LOMAC), Katholieke Universiteit Leuven (K.U.Leuven), Celestijnenlaan 200F, B-3001, Leuven, Belgium
E-mail: erik.vandereycken@chem.kuleuven.be

ABSTRACT

In the last three decades 3,5-dichloro-2(1H)-pyrazinones have emerged as useful starting materials for the elaboration of different types of skeletons of biologically interesting compounds[1]. The 2(1H)-pyrazinone scaffold allows the easy introduction of a wide range of pharmacologically active groups with the ability to address the diverse set of biological targets. We will comment on our latest results regarding the application of focussed microwave irradiation for the decoration and conversion of this useful scaffold. Our recent results about the first palladium-catalyzed desulfitative Sonogashira-type cross-coupling[2] reaction as well as concerning a desulfitative Hiyama-type cross-coupling[3] will be presented. We will also comment on the development of a novel and versatile entry to asymmetrically substituted pyrazines[4], including a microwave-assisted Liebeskind-Srogl protocol, as well as on the elaboration of an unprecedented route for the synthesis of dihydropyrazine-2,3-diones applying aqueous ("green") conditions[5]. A highly efficient method for the diversity oriented synthesis of tri- and tetrasubstituted furo[2,3-b]pyrazines has been developed comprising a Ag+- or iodine-mediated intramolecular heteroannulation reaction[6]. We will also present a new microwave-assisted palladium-catalyzed phosphonium-mediated tautomerization-activation-coupling of 2-(1*H*)-pyrazinones[7] as well as a mild room-temperature palladium catalyzed C3-arylation of 2(1*H*)-pyrazinones via a desulfitative Kumada-type cross-coupling reaction[8].

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[5] A. Sharma, V. P. Mehta, K. Van Hecke, L. Van Meervelt, E. Van der Eycken, Tet. Lett., 49, 4993-4996, 2008.
[6] D. S. Ermolat'ev, V. P. Mehta, K. Robeyns, L. Van Meervelt, E. V. Van der Eycken, Synlett, 3117-3122, 2007.
[7] V. P. Mehta, S. G. Modha, E. Van der Eycken, J. Org. Chem., 75, 976-979, 2010.
[8] V. P. Mehta, S. G. Modha, E. Van der Eycken, J. Org. Chem., 74, 6870-6873, 2009.

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Plenary Lectures

Dr. Dorothy J. Philips

Waters Corporation, Milford, MA USA

Dr. Dorothy J. Phillips earned her Bachelors of Arts in Chemistry from Vanderbilt University and her Ph.D. in Biochemistry from University of Cincinnati. She began her career at Dow Chemical Company before joining Waters Corporation in 1984. Currently she is Director, Strategic Marketing, responsible for identifying and assessing new technology and product opportunities to meet separation challenges. While in R&D she received the Manager's Award for Innovation in 1987 and 1988. In 2008 Dorothy was the first recipient of the Waters Leadership Award for outstanding contributions to Waters and the Waters Community. Dorothy has published and/or presented over 70 papers with a focus on liquid chromatography. Numerous presentations have been made worldwide at scientific symposia. Dorothy was a keynote lecturer at two recent conferences in Beijing, the IDDST conference in 2008 and at PepCon2010. She was selected to travel with the People to People Ambassador Program to China in 2004 to understand the status of the pharmaceutical sciences. The University of Cincinnati recognized Dorothy as a Distinguished Alumnus. Vanderbilt University presents annually the Dr. Dorothy Wingfield Phillips Award for Leadership. Dorothy was recognized for her outstanding achievements in and contributions to Science, the Profession, and the American Chemical Society (ACS) by being selected as a member of the 2010 Class of ACS Fellows.

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Plenary Lectures

Complete characterization of protein-based biotherapeutics using ultra-performance liquid chromatography (UPLC®) technology

Dorothy J. Phillips*, Edouard Bouvier, Paula Hong, William Warren, Ying Qing Yu, Kenneth Fountain

ABSTRACT

Complete characterization of the macromolecules derived from biological systems often requires multiple chromatographic techniques. The paradigm-changing UPLC® technology has already been proven to deliver improved chromatographic results for the analysis of biological macromolecules. UPLC derives its power from the use of columns packed with very small particles with an instrument designed and developed for these types of complex samples. In this seminar, application of this chromatographic technique to several significant bioseparations problems will be described. The characterization of glycoproteins such as monoclonal antibodies (mAb) requires analysis of the intact molecule and its glycan components. UPLC technology has now been extended to the analysis of intact proteins using a large pore size packing material with a C4 bonded phase. This column has been used to analyze a wide range of proteins including intact monoclonal antibodies. Critical for the safety of mAb therapeutics is the control of aggregates. The 1.7 μm size exclusion column for UPLC analysis of proteins gives improved resolution that leads to better accuracy when determining the % aggregates per batch. The factors in the successful use of this material for characterizing monoclonal antibodies will be reviewed. The tool for applying UPLC to the analysis of glycan structures is the 1.7 μm glycan column. This column is used for a HILIC separation of labeled glycans that are released from a glycoprotein such as mAb. UPLC technology enables the complete characterization of protein-based biotherapeutics to be less challenging.

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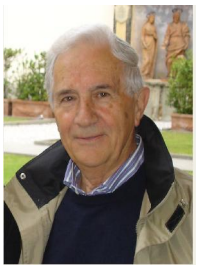
Plenary Lectures



Prof. Giampietro Sgaragli

University of Siena, Italy

Degree in Medicine & Surgery (1963); specialization in Skin and venereal diseases (1967) and Toxicology (1969) at the University of Florence.

Visiting Scientist at the Departement of Pharmacology, Yale University, U.S.A. (1972-74).

Assistant Professor in Pharmacology, Faculty of Medicine, University of Florence (1969-80).

Full Professor in Pharmacology, Faculty of Pharmacy, University of Siena (1981-2010).

Head of the Institute of Pharmacological Sciences, School of Pharmacy, University of Siena (1987-2003).

President of the Course in Pharmaceutical Chemistry and Technology, University of Siena (1990-93).

President of the course in Pharmacy, University of Siena (2000-2006).

Delegate of the Faculty of Pharmacy at the Committee for the Scientific Foreign Affairs and ERASMUS coordinator for the application of ECTS methodology, University of Siena (1994-2010).

Delegate of the Senato Accademico at the Committee for the Socrates Programme, University of Siena (1996-2010).

Referee for EC in the INTAS programme (call 1995-96 and 1996-97).

Head of the Department of Biomedical Sciences, University of Siena (2003-2006).

Delegate of MIUR to the Management Committee of COST 926 action "Impact of new technologies on the health benefits and safety of bioactive plant compounds" (2003 - 2008).

Coordinator of the Doctorate School in Physiology, in Pharmacology and Molecular and Cellular Toxicology, University of Siena (2003-2010).

Coordinator of a research project of national interest (PRIN) funded by the Ministry of University and Research (MUR) (1998), a Scientific joint project Italia-Bulgaria financed by Ministry of Foreign Affairs (MAE) (act 212/1992) and a Scientific joint project Italy-Hungary financed by MAE (act 401/1990).

Active Member of Scientific Societies in the field of Pharmacology and Toxicology.

Scientific collaborations with Biochemistry Department, Trinity College, Dublin; Departamento de Bioquimica y Biologia Molecular, Universitad Autonoma de Barcelon; MRC Bioanalytical Science Group, Birkbeck, University of London; Department of Pharmacology Oxford University; Institute of Microbiology, University of Sgezed; Department of Anaesthesiology, University of Wien; Department of Cardiovascular Physiology, University Heidelberg; Department of Human and Animal Physiology, University of Sofia; Department of Chemistry, Saurashtra University.

Fields of major interest

Metabolism and pharmacokinetic of xenobiotics; effects of synthetic and naturally occurring phenols on Ca^{2+} and K^{+} currents in vascular smooth muscle cells (patch-clamp technique); assessment of MDR reverting activity of novel compounds; modulation of vascular smooth muscle and skeletal muscle Ca^{2+} homeostasis by synthetic phenols and their protection of tissues against ischemia-reperfusion injury; neuro-pharmacology oof taurine and taurine-like compounds.

More than 160 papers in International refereed journals.

PL - 22

Plenary Lectures

In the search for novel and potent P-glycoprotein inhibitors as multidrug resistance reverting agents for cancer therapy

Giampietro Sgaragli
University of Siena, Italy

ABSTRACT

Multidrug resistance (MDR) mediated by the pumps P-glycoprotein (Pgp) and MDR-associated proteins is in most cases responsible for the clinical failure of cancer therapy with antineoplastic agents. The use of pumps inhibitors is a promising approach to overcome MDR. Among the several compounds (dihydropyridines, taxuspines…) tested so far in our laboratory, some *N,N*-bis(cyclohexanol)amine aryl esters appear promising leads for the design of effective, novel MDR reverters in cancer cells. Four geometrical isomers (a, *cis/trans*; b, *trans/trans*; c, *cis/cis;* d, *trans/cis)* characterized by *N,N*-bis(cyclohexanol)amine scaffold non-symmetrically esterified with two different aryl acids (Ar_1 = 3,4,5-trimethoxybenzoyloxy; Ar_2 = 3-(3,4,5-trimethoxyphenyl)acryloyloxy) (1a-d) were investigated as P-glycoprotein (Pgp) inhibitors by measuring cytofluorimetrically the retention of rhodamine 123 (R123) in human MDR1-gene transfected mouse T-lymphoma L5178 cells. 1a and 1d proved to inhibit Pgp with IC_{50} values much lower than those found with the most potent, established inhibitors. Since upon cell washing reversion of 1d Pgp inhibition was incomplete suggesting an irreversible binding with the target, the role of double bond present in Ar_2 was investigated inserting as Ar_2 a 3-(3,4,5-trimethoxyphenyl)propionyloxy or a 3-(3,4,5-trimethoxyphenyl)propynoyloxy moiety. Two sets of four isomers were thus obtained, where the double bond of 1a-d was substituted by a single (2a-d) and a triple bond (3a-d), respectively. 2a-d were nearly equipotent, 2d and 2c showing IC_{50} values two orders of magnitude greater than the double-bond counterparts. On the contrary, 3a-d were very effective, the most active 3d and 3c showing a potency greater than that of double-bond counterparts (1d and 1c). Concentration-inhibition curves of 1c and 3d exhibited a biphasic behaviour suggesting the existence of two binding sites for them in the recognition domain of Pgp. To probe whether the most active compounds were substrates of Pgp, R123 retention experiments were performed by using GF120918 and CSA as positive and negative controls. The persistence of inhibition of Pgp-mediated R123 cell efflux by these compounds resulted to be intermediate between that caused by CSA (a Pgp substrate) and GF120918 (a non Pgp substrate).Moreover, their inhibition of Pgp-mediated R123transport was tested at different R123 concentrations. Out of the six compounds investigated, 1d , 1c, 2d , 2c and 3c exhibited a positive cooperativity with R123 in Pgp inhibition, the inhibition-concentration curve being shifted lefttward when R123 concentration was increased, while 3d exhibited a negative cooperativity. These findings indicate that isomeric geometry and conformational freedom of Ar_2 moiety are crucial for both Pgp inhibition and their presentation to Pgp as substrate-like compounds.

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Plenary Lectures

Prof.Dr. Paul Erhardt

University of Toledo, Ohio

Paul Erhardt received a Ph.D. in medicinal chemistry from the University of Minnesota and undertook postdoctoral studies in drug metabolism at the University of Texas at Austin. His early career involved synthetic medicinal chemistry within the pharmaceutical industry. He was with American Critical Care in Chicago for 7 years as a Research Scientist, Senior Research Scientist and Group Leader. During this period he was responsible for the chemical design, synthesis and entire chemical-related pre-clinical development of esmolol, a unique 'soft drug' presently marketed as Brevibloc.® Dr. Erhardt then joined Berlex Laboratories in New Jersey as a Section Head where over the course of 11 years he became the Assistant Director of Medicinal Chemistry and, finally, the Assistant Director across all pharmaceutical R&D. To share his experiences in a formalized educational setting, Dr. Erhardt returned to academia 17 years ago by joining The University of Toledo (UT) College of Pharmacy as a tenured Professor and Director of the Center for Drug Design and Development (CD3). During this latest period he has received the College's *Outstanding Teaching Faculty Award* and *Outstanding Research Faculty Award*, as well as the University's *Outstanding Faculty Researcher Award*. Dr. Erhardt is active in the IUPAC where he has edited a book about drug metabolism considerations during drug design and development, and where he recently completed serving as President for the Division of Chemistry and Human Health. His research involves medicinal chemistry pertaining to oncology, drug metabolism and soft drug technologies, ADMET-related SAR and synergy, and chiral auxiliary synthetic reagents amenable to drug-related process chemistry. Dr. Erhardt has authored over 125 articles and patents. His annual research budget has repeatedly surpassed the 1 M dollar level and presently funds a cadre of 6 postdocs, 2 technicians and 9 graduate students.

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Plenary Lectures

Directing drug distribution: Avoiding multidrug resistance while targeting cancer cells

Paul Erhardt
University of Toledo, Ohio

ABSTRACT

Deploying paclitaxel as a scaffold, we have delineated negative structure-activity relationships (NSAR) that can be exploited to avoid the P-glycoprotein transporter that is associated to a large extent with the development of multidrug resistance (MDR) in human breast cancer cells. We also observed that the structural space encompassed by these NSAR overlapped with that which can enhance aqueous solubility and with that present in certain 'address' molecules being explored for their potential to selectively hone to cancer cells compared to normal cells. Combining these overlapping features into various hybrid attachments, we are presently synthesizing paclitaxel analogues that will simultaneously display increased aqueous solubility, enhanced selectivity for cancer cells compared to normal cells, and a significantly decreased liability for the development of MDR. While elaborating the specific chemistry associated with the preparation and optimization of the various address system partners, we are also incorporating cargos that can be used as biochemical probes (dyes and quantum dots) and as contrast enhancing agents for diagnostic imaging (ultrasound).

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Plenary Lectures

Prof. Janine Cossy

Professor of Organic Chemistry, Laboratoire de Chimie Organique, ESPCI ParisTech, 10 rue Vauquelin 75231 Paris Cedex 05

Academic Record

1974: Master in Chemistry, University of Reims (France)
1976: Thèse de 3eme cycle (Supervisor: Pr J. P. Pète, Université de Reims, France)
1979: Doctorat ès Sciences Physiques (PhD Supervisor: Pr J. P. Pète, Université de Reims, France)
1980-1982: Postdoctoral position with Pr B. M. Trost, University of Wisconsin (MADISON, USA)

Employments

1976-1990: CNRS research assistant in Reims
1st October 1990: CNRS director of research in Reims
2nd of October 1990-present: Professor at ESPCI in Paris (Ecole Supérieure de Physique et Chimie Industrielles de la Ville de Paris)
1992-present: Director of a CNRS Reseach Unity

Field of research

Photochemistry, thermal reactions, radicals, rearrangements, enantioselectivity, organometallic chemistry, catalysis, synthesis of natural products and/or biologically active compounds.

Scientific activity

- 357 publications in international journals + 4 publications submitted
- 13 Patents
- 16 Book chapters
- Edition of 4 Books + 3 books in preparation
- 350 invited conferences

Among the Awards, Scholarships and Honours

1987: CNRS Bronze Medal (France)
1996: Jungfleish Award from Académie des Sciences (France)
1996: CNRS Silver Medal (France)
1997: Chevalier de l'Ordre du Mérite (France)
2005: UK Royal Society Rosalyn Francklin International Lecturership awarded to internationally recognized women scientists (UK)
2009: Le Bel Award from the French Chemical Society (France)
2010: Royal Society Chemistry RSC/SFC Award. European Lecturership in the Chemical Sciences (UK)
2010 : Astra Zeneca Lecturership (Stockholm, Sweeden)

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Plenary Lectures

Catalytic reactions access to biologically active complex molecules

Janine Cossy
Laboratoire de Chimie Organique Associé au CNRS, ESPCI*ParisTech*, 10 rue Vauquelin, 75231 - Paris Cedex 05, France

ABSTRACT

Complex biologically active molecules are a good source of inspiration to develop methods as one of the major challenge, in synthetic organic chemistry, is the design and execution of concise approaches to these molecules. Strategies that are using reactions that rapidly lead to the skeleton framework of natural and/or biologically active compounds are attractive. In the context of developing facile entries to biologically active compounds possessing complex structures, we have explored their construction using catalytic reactions involving organometallic, organic catalysts, enzymes to induce coupling reactions, diastereoselective cyclizations and enantioselective condensations. These methods and their applications to the synthesis of biologically active complex natural and non-natural compounds will be presented.

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Plenary Lectures

Prof.B. P. Bandgar

Vice Chancellor, Solapur University, Solapur-Pune Highway, Kegaon, Solapur-413255, Maharashtra, India.
Tel. : 091-217- 2351300; Fax : 091-217- 2351300
E-mail : bandgar_bp@yahoo.com; Url: http://su.digitaluniversity.ac

Qualification

M.Sc. M.Phil. Ph.D. (Vienna, Austria)

(i) S. S. C to B.Sc. First Class With Distinction, M.Sc. First Class, M.Phil. in 'A' grade.
(ii) B.Sc.(Chemistry), M.Sc. (Organic Chem), M.Phil. (Synthetic Organic Chem.) Shivaji University, Kolhapur, Maharashtra.
(iii) Ph. D. (Medicinal Chem.) : University of Vienna, Austria, Europe

Teaching Experience

30 years
18 Years in Rayat Shikshan Sanstha.
10 Years in Swami Ramanand Teerth Marathwada University, Nanded.
02 Years at Solapur University, Solapur.

Research areas of Interest

1. Development of Novel Synthetic Methods in Organic Chemistry.
2. Carbohydrate Chemistry.
3. Medicinal Chemistry
4. Synthesis of Bioactive Molecules.

Awards, Honors, Scholarships and Fellowships

(i) Indian Govt. Merit Scholarship throughout the University Education.
(ii) UGC New Delhi: Teacher fellowship for M.Phil.
(iii) Austrian Govt. fellowship (OAD) for Doctorate degree at University of Vienna.
(iv) Young Scientist award (ICC): 1994.
(v) Fellow of Maharashtra Academy of Sciences: January 2003.
(vi) UGC visiting fellow
  a. Sardar Patel University, Vallabh Vidyanagar, Gujrat 2006 and 2007.
  b. Rashtrasant Tukdoji Maharaj Nagpur University, Nagpur: 2006-07.
(vii) Excellent Teacher award of State Govt. of Maharashtra : September 2006
(viii) Fellow of Indian Chemical Society.
(ix) Life member of Indian Council of Chemists.
(x) Fellow of American Chemical Society, USA.
(xi) Tetrahedron Letters Award (USA) for most cited paper during 2003-06: Sept 2006.
(xii) Lok Raja Shahu Maharaj Award – 2008.
(xiii) Vivekaknd Puraskar – 2008.
(xiv) Sangola Ratna – 2008.

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Plenary Lectures

Chemistry, biology of novel anti-inflammatory and anti-cancer agents

B. P. Bandgar
Vice-Chancellor Solapur University, Solapur-413 255, M. S.

ABSTRACT

With the advent of combinatorial chemistry, the number of new chemical entities (NCEs) can be produced in a short space of time by drug discovery teams. Although this has produced a wealth of possible new therapeutic compounds, it has also raised an important question about screening of most therapeutically active ons, from thousands of compounds. One approach to solve this problem has been th us of in vitro screens to identify the characteristics of an NCE, particularly with respect to its drug metabolism. Such information is crucial to the decision making process of which compounds to progress with and which to discard. Such an approach can also be used to screen smaller sets of structurally related compounds, allowing determination of the chemical structure that is the strongest possible lead candidate.

Increased generation of reactive oxygen species (ROS) has been observed in cancer, degenerative diseases and other pathological conditions. ROS can stimulate cell proliferation, promote genetic instability and induce adaptive responses that enable cancer cells to maintain their malignant phenotypes. However, when cellular redox balance is severely disturbed, high levels of ROS might cause various damages leading to cell death. Cancer is the second leading cause of in the present society after cardiovascular diseases. A great deal of efforts have been underway to treat various forms of cancer for decades; and until recently, chemoprevention of cancer is receiving its due to share of attention. Combinatorial chemistry and high-throughput screening against pure molecular targets and cancer cells are established methods for primary anticancer drug discovery.

Inflammation is the body's way of dealing with infections and tissue damage, but there is a fine balance between the beneficial effects of inflammation cascades and their potential for long-term tissue destruction. If they are not controlled or resolved, inflammation cascades can lead to the development of diseases such as chronic asthma, rheumatoid arthritis, multiple sclerosis, inflammatory bowel disease and psoriasis. Within many inflammation cascades or pathways, there are often pivotal molecular targets that, when antagonized or neutralized, block the output of the pathway. A relatively small number of pivotal targets has been identified that have yielded many successful anti-inflammatory drugs. These targets include the enzymes (COX 1 and COX 2), cytokines (tumor necrosis factor-α , interleukin-6 and interleukin-2) and the receptor for the cysteinyl leukotrienes C4 and D4 and nuclear membrane receptors (corticosteroids). Therefore, inhibition of these targets has become a major focus of current drug discovery and development, and an important in vitro method for evaluating the bioactivity of drugs.

Some recent work carried out by the author on anti-inflammatory and anticancer drug molecules [1-9] will be presented in the conference.

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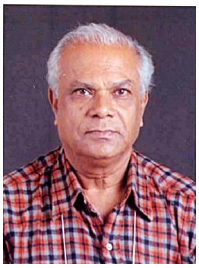
Plenary Lectures



Prof. H.Junjappa

Reva- Institute of Science and Management, Kattigenahalli,Yelahanka, Bangalore-560064.
E-mail: Junjappa-123@rediffmail.com

H.Junjappa was born on 23rd May, 1936 in Aladgeri village, Taluk: Hirekerur, Dharwar Dist. in Karnataka state. He received his B.Sc. (1958) and M.Sc degree (1960) in chemistry from Karnataka University, Dharwar and continued research in the same university in organic chemistry under the guidance of Prof.S.Siddappa and received his Ph.D degree in 1964. he than worked as postdoctoral fellow at Department of Chemistry, IIT, Kanpur under Professor M.V.George (1965-1967) and moved subsequently to Ohio State Uni., Columbus, USA as postdoctoral fellow to work with

Prof. M.S. Newman (1967-1969). He then worked as a postdoctoral fellow in Texas Tech. University, Lubbock under Professor H.J.Shine (1969-1970). He returned to India initially to join as pool officer (CSIR) at Central Drug Research Institute, Lucknow (1970) and subsequently joined there as scientist in the Medicinal Chemistry Division (1971-1976). He then moved to newly established North Eastern Hill University, Shillong as a founder Head to start the new Chemistry Department and continued there till his retirement in 1998. later he joined as emeritus scientist (CSIR) at Department of Chemistry at IIT Kanpur (1998-2001) and subsequently moved to Bangalore in 2002 and established a custom research company called; Biooganic and Applied Materials Ltd;. As founder director (2002-2005). He is now settled in Bangalore.

He began his research career at CDRI Lucknow, where he developed a versatile synthetic chemistry involving α-Oxoketenedithioacetals as 1, 3-dielectrophilic building blocks, which on reaction with a variety of 1, 2 and 1, 3-dinucleophiles to yield biologically important 5 and 6 membered heterocycles. His contribution on aromatic annulation has evolved into the name reaction. "The Junjappa-Ila(JI) Aromatic and Heteroaromatic Annulation".

Over 55 students have received Ph.D degree under his supervision and published more than 220 research papers. Delivered R.C Shah Memorial lecture (1995), T.R Sheshadri memorial lecture (1996), 4th Dr. Sukh Dev endowment lecture (1996) and visiting professor, Ibedrola national foundation Spain in Savilla (1999). He is a Fellow of Indian Academy of sciences Bangalore and Indian National Science Academy, New Delhi. Currently Prof. Junjappa is a research professor in Reva Institute of Science & Management, Yelahanka, Bangalore – 64.

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Plenary Lectures

The Junjappa-Ila(JI)- Aromatic and hetro aromatic annulation. Universal synthetic strategy for benzo and condensed hetrocycles

H. JUNJAPPA
Reva- Institute of Science and Management, Kattigenahalli,Yelahanka, Bangalore-560064.
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ABSTRACT

In recent years [3+3] benzoannulation reactions have become the subject of intense investigation primarily due to easy availability of both 1, 3- dielectrophilic and the corresponding di nucleophilic symthoms. The α- 0xoketene dithioacetals, and a variety of their structural analogs, react with allyl/ and hetero allyl anions,- to yield, benzenoids, condensed aromatics benzoheterocycles in good to excellent yields. The scope and limitations of this aromatic/ heteraromatic annulation protocol will be discussed.

REFERENCES

[1] Review: Junjappa H., lla H., Mohanta, P.K. Progress in Heterocyclic Chemistry; Gilchrist, T.L. and Gribble, G.W.Eds.; Pergamon Press, Vol. 13, 2001, p.1.
[2] Review: Junjappa H., lla, H., Asokan, C.V. Tetrahedron, 1990,46,5423.
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[5] Review: Katritzky, A.R., Li, J., Xie, L. Tetrahedron, 1999, 55, 8263.
[6] Kumar, s., Ila, H., Junjappa, H. tetrahedron, 2007,63,10067 and references therein.

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Plenary Lectures

Dr. Tina M. Nenoff

Distinguished Member of Technical Staff, Surface and Interface Sciences Department, Sandia National Laboratories, PO Box 8500, MS 1415, Albuquerque, NM 87185 USA
Tel: 505-844-0340; Fax 505-844-5470
E-mail: tmnenof@sandia.gov

Education / Training

University of California, Santa Barbara	MS/PhD	1988-1993	Chemistry
University of Pennsylvania	BA	1983-1987	Chemistry

Professional Positions

2002-present	Distinguished Member of the Technical Staff, Sandia National Laboratories
1997-2002	Principal Member of the Technical Staff, Sandia National Laboratories
1993-1997	Senior Member of the Technical Staff, Sandia National Laboratories
1987-1988	Research Associate, Ciba-Giegy Chemicals, Ardsley, NY

Tina Nenoff is a Distinguished Member of the Technical Staff at Sandia National Laboratories in Albuquerque, NM. She established her research there after receiving her Ph.D. in Chemistry from the University of California, Santa Barbara under the guidance of her advisor Dr. Galen Stucky. Her current research interests are in the structure/property relationships of novel nanoporous and nanoparticle phases. Research areas of interest include: novel materials for the removal and fixation of radioisotopes and elements; novel nanoparticle phase formation via radioloysis; and inorganic thin film membranes for light gas and organic molecule separations and catalysis.

She is a member of American Chemical Society (ACS), Material Research Society (MRS) and International Zeolite Association (IZA); and holds leadership positions in both the ACS and IZA. She is chair for the 2011 Nanoporous Materials Gordon Research Conference. She is member of the editorial board of *Chemistry of Materials*, co-editor *MRS Bulletin* (10/06), and a reviewer for numerous journals. Dr. Nenoff has published 125+ papers in various material science and chemistry journals, holds 9 US Patents and has presented at over 100 national and international conferences.

Plenary Lectures

Novel materials involved in radiological environments

Tina M. Nenoff
Surface and Interface Sciences Dept., Sandia National Laboratories, Albuquerque, NM USA

ABSTRACT

We are interested in the structure/property relationship between materials on their nanoscale and their bulk properties. We are also interested in new materials either made by or made for radiological environments, which many times involves the accessing of phase spaces that are different from traditional materials. Two overview examples of this research are described in this presentation: porous frameworks for the separation and storage of volatile gases and the room temperature synthesis of nanoparticle alloys,.

Part 1: The effective capture and storage of radiological iodine (129I) remains a strong concern for safe nuclear waste storage and safe nuclear energy. Silver-loaded mordenite (MOR) is a longstanding benchmark for iodine capture (chemisorbed as AgI). Metal organic frameworks (MOFs) and Ag-MOFs are a natural extension of the zeolite research. However, the molecular level understanding of this process needed to develop more effective iodine getters has remained elusive. Here we probe the structure and distribution of iodine sorbed by silver-loaded MOR and various metal organic framework systems using differential pair distribution function (PDF) analysis. We will present detailed descriptions of the materials synthesis, characterization, differential PDF, and associated models necessary for determination of the structure-property relationship of these phases.

Part 2: Bimetallic nanoparticles (NPs) have attracted tremendous interest currently due to their special optical, catalytic, electronic/magnetic, and Hydrogen interaction properties. All these properties can be greatly affected by the structures of bimetallic NPs, i.e. alloy vs. core-shell. However, using radiolysis, we were able to synthesized stable, homogenous metal, bimetallic and alloy NPs via a radiolytic approach. The reaction required the gamma-irradiation of an aqueous solution of individual metal salts and organic stabilizing molecules. The irradiation produced a large concentration of reducing electrons, which directed the chemistry of the NP formation. We have successfully synthesized AgNi and PdNi NPs at room temperature. We have employed UV-vis, HRTEM, HAADF-STEM imagine, single particle EDX and EFTEM mapping characterization techniques to confirm the composition and alloying of these NPs. Furthermore, we confirmed the AgNi NPs are stable and did not experience dealloying process upon heating.

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Plenary Lectures

Dr. Françoise Pontet

Service de Biochimie et Biologie Moléculaire, Hôpital Lariboisière,
2 rue A Paré, 75475 Paris, France
E-mail : francoise.pontet@free.fr

Dr. Françoise Pontet is Chair of the joint Committee-Subcommittee on Nomenclature for Properties and Units (C-SC-NPU) of the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC) and IUPAC, and Vice-President of IUPAC Division VII-Chemistry and Human Health. She coordinates the C-SC-NPU activities, which are centered around the maintenance of the NPU terminology, which aims at providing a standardized format for the electronic transmission of requests and results of Clinical Laboratory examinations. She is also the IFCC representative to the Joint Committee for Guides in Metrology-Working Group 2 and as such contributes to elaborate the International Vocabulary of Metrology (VIM).

Dr. Pontet graduated from Paris University, college of Pharmacy as a Pharmacist, specialized in human biology, with postgraduate degrees in Hematology, Parasitology and Biochemistry. She earned her PhD on monoclonal IgM and search of malignancy criterium. She earned an award in Parasitology and a thesis award. She completed her internship at the Hôpital Lariboisière, Paris. Then, she supervised the protein section of the biochemistry department during 22 years. She has been an active member of the Société Française de Biologie Clinique (SFBC), and President of its Committee on Proteins. She conducts epidemiology works on monoclonal immunoglobulins.

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Plenary Lectures

Health informatics: The NPU coding system

Françoise Pontet*
On behalf of the Joint IFCC-IUPAC Committee on Nomenclature for Properties and Units.
***Service de Biochimie et Biologie Moléculaire, Hôpital Lariboisière, 2 rue A Paré, 75475 Paris, France**
E-mail : francoise.pontet@free.fr

ABSTRACT

In clinical laboratory sciences a nomenclature is required to facilitate electronic exchanges. C-NPU provides a database of standardized terms which is structured according to SI, ISO, IUPAC and IFCC recommendations.

The NPU terminology is developed by a joint IFCC-IUPAC committee (C-SC-NPU). Standardized requests and reports of clinical laboratory results have the following syntax: which part of the universe (System), which component in that part (Component), which component property (kind-of-property) are examined, and result (= ? unit). Specifications can be added. The resulting syntax is :

System(specification)—Component(specification);kind-of-property(specification) = ? unit

This work shows the interesting aspects of the C-NPU coding system : a multilingual terminology set (9 language versions), patient centered and constantly revised according to scientific advances. The English version is freely accessible and downloadable for any biologist worlwide through the Internet, at <http://www.sst.dk/English/NPULaboratoryTerminology.aspx>. SI units are provided. Component terms refer to authorized sources. It is simple and unique as all terms are directly provided by the database for each situation and adapted to it. The C-NPU database includes 15 000 terms covering all fields of clinical laboratory sciences, each with a specific and ready-to-use code. Mapping of NPU coding system to SNOMED CT is being performed.

Examples of the contents of this terminology are presented in the communication.

The background for the IFCC-IUPAC coding system for laboratory investigations is described in the publications listed at (http://old.iupac.org/divisions/VII/labinfo/English/IFCC_Documents.html).

Using the C-NPU coding system brings a considerable progress in the electronic communications of clinical laboratory sciences.

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Plenary Lectures

Prof. Rolf Breinbauer

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Fax: +43 316 873 32402
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Work Experience

since 2007 Full Professor and Director of the Institute of Organic Chemistry
Graz University of Technology
Graz, Austria

2005 - 2007 Professor of Organic Chemistry
University of Leipzig
Leipzig, Germany

2003 - 2005 Junior-Professor of Bioorganic Chemistry
University of Dortmund
Leipzig, Germany

2000 – 2006 Group Leader, Department of Chemical Biology
Max-Planck-Institute of Molecular Physiology,
Dortmund, Germany

1998 - 1999 Post-doctoral Fellow, Department of Chemistry (Prof. E. N. Jacobsen)
Harvard University, USA

1995 - 1998 Research Assistant (Ph.D. student),
Max-Planck-Institute of Coal Research (Prof. M. T. Reetz)
Mülheim/Ruhr, Germany

Education

1995 - 1998 Ph.D. dissertation (grade "summa cum laude"):
"Metal Colloids as Catalysts"
MPI Mülheim & University of Bochum, Germany

1989 - 1995 Diploma in Technical Chemistry
Vienna University of Technology, Austria

1994 - 1994 ERASMUS-student, work on diploma thesis
University of Heidelberg (Prof. G. Helmchen)
Heidelberg, Germany

1989 Matura (grade: "with distinction"),
Bundesgymnasium Schärding, Austria

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Plenary Lectures

Synthesis of tool compounds for chemical biology

Rolf Breinbauer
Institute of Organic Chemistry, Graz University of Technology, Stremayrgasse 9, A-8010 Graz
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ABSTRACT

In my presentation I will report about two aspects of research in our group. The first part deals with the synthesis of compound libraries which can be used in Chemical Genetics screen. Within this part I will cover our contributions in combinatorial solid phase synthesis[1] and a collaborative effort for preparing small molecule arrays for high content screening[2]. In the second part of my talk I will present our efforts in the structured guided synthesis of tool compounds to study protein function. In particular, I will report about our common studies with the Blankenfeldt laboratory to investigate the biosynthesis of phenazines – a well known bacterial virulence factor[3]. In this endeavour we identified the first protein ligand which binds with both enantiomers at the same time to a protein.[4]

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[2] Köhn, M., Gutierrez-Rodriguez, M., Jonkheijm, P., Wetzel, S., Wacker, R., Schröder, H., Prinz, H., Niemeyer, C. M., Breinbauer, R., Szedlacsek, S., & Waldmann, H. (2007). Angew. Chem. Int. Ed. 2007, 46, 7700-7703.
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PL - 32

Plenary Lectures

Prof.Indrapal Singh Aidhen

Professor, Department of Chemistry, Indian Institute of Technology-Madras, Chennai 600 036, India
Tel: +91-44-22574219
E-mail: isingh@iitm.ac.in

Education

B. Sc. Poona University, Pune (1981)
M. Sc. Poona University, Pune (1983)
Ph. D. Department of Chemistry, University of Poona, Pune (1990)

Research Experience

Hoechst Research Center, Mumbai, India (1983-1985)
National Chemical Laboratory, Pune, India (1991-1992) as Fellow Scientist
University of California, Santa Cruz, USA (04/1992 - 04/1993) as Post-Doctoral Fellow
University of Konstanz, Germany (12/1993 – 04/1995) as Post-Doctoral Fellow
IIT-Madras, India (12/1995 – Present) as Faculty

Research Interests

Synthesis of Biologically Important Molecules
Synthetic Carbohydrate Chemistry
Developing New Building Blocks based on Weinreb-amide Functionality

Honors and Award

Rated High as a Teacher at IIT-Madras
Alexander von Humbolt Fellowship Award, Germany (1993)
JSPS-Invitation Fellowship Award, Japan (2003)
Visiting Auxiliary Faculty, University of Utah, USA (2001)
National Merit Scholarship Award, India (1981)

Achievements

Publications	42	Patents	03
Ph. D.s	06 (completed) 05 (on-going)	M. Sc-Projects	15

Weinreb-Amide based Building Block developed at IIT-Madras finds place in Aldrich Catalogue [*Catalogue compound No: 56, 108-8*]

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Plenary Lectures

Synthesis of FTY720 and novel C-glycosylated phenstatin analogues using weinreb amide based building blocks

Indrapal Singh Aidhen*
Department of Chemistry, Indian Institute of Technology-Madras, Chennai-600036, INDIA
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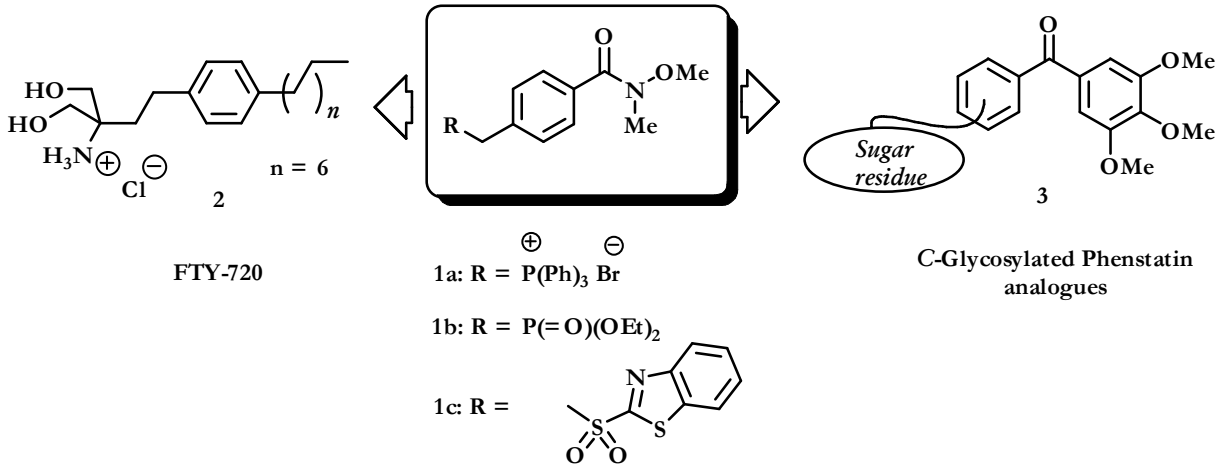
ABSTRACT

Our continued interest in developing building blocks based on Weinreb-amide functionality towards application in the synthesis of challenging and important targets has enabled development of three new building blocks 1a-1c.[1] Initially it paved way for an efficient synthesis of FTY720, recently approved drug for multiple sclerosis and later laid the grounds for arriving at C-glycosylated phenstatins 3, novel analogues of phenstatins as promising anti-mitotic agents. The lecture will focus on the strategy developed for an efficient and convenient synthesis of 2[2] and 3.[3]



REFERENCES

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[2] Sivaraman, B.; Senthilmurugan, A.; Aidhen, I. S. Synlett 2007 2841.
[3] Sivaraman, B. Aidhen, I. S. Eur. J. Org. Chem. 2010, 4991.

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Plenary Lectures

Prof.Graham Jones

Professor, Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA, USA

Graham B. Jones is Professor and Chair of Chemistry & Chemical Biology and Co-Director of the Barnett Institute of Chemical & Biological Analysis at Northeastern University in Boston, Massachusetts, USA. Jones was educated in the UK, receiving BSc and PhD degrees in chemistry from the University of Liverpool and the Imperial College of Science Technology and Medicine respectively. He then moved to the USA as a NATO fellow and conducted independent research at Harvard University with E. J. Corey, the 1990 Nobelist in chemistry. His research expertise lies at the interface of organic and medicinal chemistry, and has resulted in over 120 publications, generated in excess of $10M external funding and forged numerous collaborative partnerships with the pharmaceutical and biotechnology industry. He has been appointed to several editorial posts for scholarly scientific journals, and was awarded the DSc degree in 2006 for his contributions to medicinal chemistry. Graham has held a variety of influential executive positions in the academic sector both in the UK and USA, including Pro-Vice Chancellor at the University of Hull

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Plenary Lectures

Expedited synthesis of fluoroalkyl and fluoroarene radiopharmaceuticals for PET imaging

Graham B. Jones
Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA, USA

ABSTRACT

PET and SPECT have become significant imaging modalities for the analysis of oncologic, cardiovascular and CNS disorders, providing the potential to track metabolic pathways which can compliment the anatomical images provided by magnetic resonance methods. The need for rapid introduction of short half-life radio nuclides for use in SPECT and PET imaging presents an ideal application for microwave mediated organic synthesis. Microwave chemical reactors have now evolved to the degree that desktop chemical syntheses can be performed with considerable precision, the microwave method of thermolysis having a substantial accelerating effect on chemical reactions and typically minimizing formation of unwanted byproducts. Using commercially available systems we have developed a number of versatile and proprietary methods for the introduction of ^{18}F, ^{123}I, ^{125}I and other labels to drug candidates for subsequent in vivo imaging. The benefits of the Northeastern methods include speed (~5 min reaction time) and clean up – giving rise to extremely pure compounds following simple cartridge filtration. The methods can be applied to introduce the radiolabel either on an alkyl chain or directly on an aromatic (or heteroaromatic) ring. The scope of the processes is noteworthy, and we are currently demonstrating applications in the synthesis of FDA approved drugs so that biodistribution studies can be conducted. These include the anti-psychotic agents haloperidol and risperidone the nAChR ligand 5IA-85380, the nicotinic [$\alpha_4\beta_2$] receptor agonist nifrolidine, and the cardiovascular imaging agent RP1005.

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Plenary Lectures

Dr. Zafra M. Lerman

President, MIMSAD, Inc., 1911 Grant Street, Evanston, IL 60201 USA
Tel: (847) 866-7299

Zafra Lerman is the President of MIMSAD (Methods Integrating Music, Science, Art and Dance). Her Ph.D. is from the Weizmann Institute of Science, Israel, and she conducted research at Cornell and Northwestern Universities, and the ETH, Zurich, Switzerland.

She developed an innovative approach of teaching science at all levels using the arts and cultural backgrounds, which received international recognition, and she has lectured around the world.

For 25 years, she has chaired the Committee on Scientific Freedom and Human Rights for the American Chemical Society (ACS). At great risk to her safety, she was successful in preventing executions, releasing prisoners of conscience from jail and bringing dissidents to freedom.

Since 2001, she has been using chemistry as a bridge to peace in the Middle East. She chairs the organizing committee for the "Malta Conferences" which bring together scientists from 14 Middle East countries with six Nobel laureates to work on solving regional problems, establishing cross-border collaborations, and forging relationships that bridge chasms of distrust and intolerance.

Prof. Lerman has received 38 international awards for her work such as the Presidential Award from President Clinton (1999); the World Cultural Council's World Award for Education in Johannesburg, South Africa (2000, the first international award in the new democratic South Africa); the ACS Parsons Award for outstanding public service to society through chemistry (2003); The Royal Society of Chemistry, England, Nyholm Education Award (2005); New York Academy of Sciences Pagels Human Rights Award (2005); George Brown Award for International Scientific Co-operation CRDF, established by the U.S. Congress; the ACS Pimentel Award for excellence in chemical education (2010); and the Peace Award from the International Center for Innovation in Education (2010).

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Plenary Lectures

Using chemistry to bridge gaps between nations

Zafra M. Lerman

ABSTRACT

My research on isotopes and my teaching environmental science made me worry about our future, our planet, and our safety and security. I realized that my worries ultimately stemmed from our dependence on oil and on the Middle East. The Middle East is a region that has been in conflict for many years. This part of the world is of particular importance because it has a source of energy that is a strategic resource: fossil fuel. This non-renewable source of energy is not only fueling economic and political conflicts, but its world-wide use is also placing at risk the sustainability of life on Planet Earth, by polluting the environment and contributing to climate changes. The Middle East also has major problems of air and water quality, which require regional cooperation. Geopolitical borders are only lines on a map; air and water do not recognize these lines. Therefore, any work concerning the environment must be done in collaboration between nations. Chemistry is an international language. A chemist from Bethlehem, Pennsylvania in the USA, and a chemist from Bethlehem, Palestine, use the same chemical notations, and can communicate scientifically to one another without understanding each other's spoken language. Building on the international language of chemistry, we developed the biannual international "Malta Conferences", which use chemistry as a bridge to peace. Scientists from 14 Middle East nations gather with six Nobel laureates to attend workshops on air and water quality; energy resources; medicinal chemistry; nanotechnology and material science; and chemical education and green chemistry. These conferences have spurred collaborations between the scientists and have yielded results that are a cornerstone for a bridge to peace.

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Plenary Lectures

Prof. Virendra Nath Pandey

Department of Biochemistry and Molecular Biology, New Jersey Medical School, UMDNJ, Newark, NJ 07103
Tel: 973-972-0660; Fax: 973-972-8657
E-mail: pandey@umdnj.edu

Education

1963-68: B.Sc and M.Sc (Mycology and Plant Pathology) Banaras Hindu University, India
1983-85: Ph.D. (Biochemistry), University of Bombay, India

AWARDS AND HONOR

1991 Shanti Swaroop Bhatnagar Prize in Life Sciences awarded by Prime Minister of India.
1992 Biotechnology Associateship, Awarded by the Department of Biotechnology, Government of India
2003 Invited chair "Reverse Transcription Session" Retroviral Meeting, Cold Spring Harbor Laboratories, New York
2005 Invited Speaker "Plenary Lecture" International Symposium on Recent Trends in Drug Discovery Indian Society of Chemists and Biologist, Saurastra University, India
2006 International Advisory Board, International Conference on Drug Discovery, Central Drug Research Institute, Lucknow, India
2007 Invited Speaker, 3rd Annual Meeting of Oligonucleotide Therapeutic Society BERLIN, GERMANY, October 2007
2008 Invited speaker "Plenary Session" International Conference on the Interface of Chemistry-Biology in Biomedical Research Feb 2008, at Birla Institute of Science and Technology, Pilani, Rajasthan.
2008 Invited Chair "Anti HIV-1 Drug Development Session" October 2008, International Drug Discovery Science and Technology BEIJING, CHINA
2009 Invited speaker, 36th Annual Meeting of Control Release Society, Copenhagen, Denmark, July 18-22, 2009

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Plenary Lectures

Proteomics of hepatitis C virus - Host cell interaction: Identification of cellular/viral factors associated with HCV (+) strand RNA genome

Nootan Pandey, Alok Upadhyay and Virendra N Pandey*
Department of Biochemistry and Molecular Biology, UMDNJ-New Jersey Medical School, 185 South Orange Avenue, Newark, NJ 07103
E-mail: Pandey@umdnj.edu

ABSTRACT

Chronic infection by Hepatitis C virus (HCV) is the leading cause of severe hepatitis which often develops into liver cirrhosis (LC) and hepatocellular carcinoma (HCC). HCV preferentially replicates in hepatocytes without any direct cytopathic effect and thus able to maintain persistent chronic infection. The molecular mechanisms underlying HCV replication and pathogenesis are poorly understood. Similarly, the role(s) of host factors in the HCV replication and associated pathogenesis remain undefined. It is likely that a number of cellular factors may be involved in facilitating HCV replication and establishing chronic infection and its subsequent progression to LC and HCC. However, the identity of cellular factors interacting with HCV RNA genome is largely unknown. Recently a number of cellular proteins interacting with *in vitro* transcribed HCV 3'NTR have been affinity captured and identified by LC/MS/MS; some of these proteins were found to be critical for HCV replication as validated by siRNA (Harris et al., 2006). A more direct approach would be to capture the replicating HCV RNA genome *in situ* and identify all the associated cellular and viral factors. The structured HCV genome and the interplay of tightly regulated viral and host factors assembled on it should be highly specific and relevant. In the present talk, we present a novel strategy to capture the replicating HCV genome from HCV infected cells and have identified associated cellular/viral proteins by state-of-the-art proteomics technology.

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Plenary Lectures

Prof.Ramaiah Muthyala

Research Associate Professor, Medicinal Chemistry, Pharmacy,
Member, Center for Drug Design
Tel: (612) 624-7120
E-mail: muthy003@umn.edu

Education

Ph.D., University of Sagar, India, 1968
Ph.D., University of East Anglia, England, 1975

Research Interests

The direction of Dr. Muthyala's research program is to focus on biological and chemical information to transform biologically active molecules into useful drugs. The drug design process will combine:

- Structural information from proteins
- Enzyme studies using computer modeling
- Synthetic methods to build molecules

Antibacterials

Over the last two decades, drug resistant strains of bacteria have increased, while the discovery and design of new and effective antibacterial agents by the drug industry have not kept up pace. Our focus is to identify novel chemotherapeutic agents based on well-recognized cell wall biosynthetic processes of the bacterial life cycle. Of great concern is the emergence of resistant bacterial strains to vancomycin, the last line of defense against severe infection, especially when all else fails. Our strategy is to design an antibiotic that will overcome this resistance and become a replacement for this drug.

Neurological Disorders

The cholinergic hypothesis states that Alzheimer's Disease is caused by the poor functioning of acetylcholine, a brain chemical important for learning and memory. This hypothesis has led to perhaps the only successful drug treatment for Alzheimer's Disease, using molecules which block acetylcholinesterase, a protein which processes acetylcholine. We are therefore searching for novel, potent, and selective inhibitors that target acetylcholinesterase.

Neuro-degeneration in Alzheimer's may be caused by the deposition of amyloid protein in brain tissue. The amyloid precursor protein is converted to amyloid protein by a-, b-, and g- secretases. Recent advances in the study of secretases have allowed us to propose selective inhibitors that might block formation of the amyloid protein.

Honors and Awards

Fellow of Royal Society of Chemistry, UK; S.C.Amita Award from Indian Chemical Society

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Plenary Lectures

Discovery of therapeutics for the spinocerebellar ataxia type 1 (SCA1)

Ramaiah Muthyala
Department of Experimental Clinical Pharmacology, University of Minnesota, Minneapolis, MN 55455, USA
E-mail: muthy003@umn.edu

ABSTRACT

Spinocerebellar ataxia type 1 (SCA1) is a fatal neurodegenerative disorder usually presenting in the third or fourth decade. The part of the brain associated with coordinating movement breaks down; interrupting walking, speech, and eventually even swallowing. There is currently no treatment or cure for SCA-1, although stem cell research may offer solutions in the future. It is caused by a CAG triplet repeat expansion that leads to a polyglutamine expansion mutation in the ataxin-1 protein. SCA1 first presents with gait abnormalities and progresses to widespread dysfunction of the cerebellum and brainstem, eventually leading to death ten to fifteen years after onset. Our ultimate goal is the development of effective treatments for SCA1, which has an incidence rate just under 1 in 100,000. Studies show that at least three things are necessary for SCA1 pathology: an expanded polyglutamine repeat on ataxin-1, entry of ataxin-1 into the nucleus, and phosphorylation of ataxin-1. The focus of the presentation is the phosphorylation of ataxin-1 as a therapeutic target.

REFERENCES

[1] Srinivasarao Yaragorla and Ramaiah Muthyala; Concise total synthesis of cytotoxic natural products (+) and (-)-muricatacin; ARKIVOC, 2010, X, p178 -184
[2] Formal total synthesis of (-)-balanol: a potent PKC inhibitor, Srinivasarao Yaragorla and Ramaiah Muthyala, Tetrahedron Letters, 2009, 51, 467-470

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Plenary Lectures

Prof. Karol Grela

Institute of Organic Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224, Warsaw, Poland; Organometallic Synhesis Laboratory, Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093, Warsaw, Poland
Url: http://www.karolgrela.eu/

Karol Grela was born in Warsaw, Poland in 1970. He received Master degree from Warsaw University of Technology in 1994, and received his Ph.D. degree from *Institute of Organic Chemistry, Polish Academy of Sciences*, in 1998. After receiving a great deal of scientific motivation from his supervisor, Professor Mieczysław Mąkosza, he moved for a postdoctoral research to *Max-Planck-Institut für Kohlenforschung*, Mülheim an der Ruhr, Germany, just in time to be present at the blooming of metathesis methodology in the labs of Professor Alois Fürstner. Next, he returned to Warsaw and after completing Habilitation in 2003 he was promoted to Associate Professor at the *Institute of Organic Chemistry, Polish Academy of Sciences* where he leads a small but very efficient research group of dedicated co-workers. His synthetic research focuses on improving synthetic efficiency, organometallic chemistry and catalysis, as well as their application to the synthesis of natural products and pharmaceutically relevant compounds. His work with metals involves the development of new catalysts and conditions for alkene and alkyne metathesis. He has published fifty manuscripts, holds six patents or patents pending and has given a number of invited international lectures. He consults for a number of companies and collaborates directly with many academic and industrial laboratories. Dr. Grela was awarded the *Alexander von Humboldt Fellowship* (1999), the *Włodzimierz Kołos Prize* (2003) and the *Prime Minister of Polish Government Prizes* (1999 and 2004).

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Plenary Lectures

Motivational tools in challenging olefin metathesis reactions

Karol Grela[1,2]

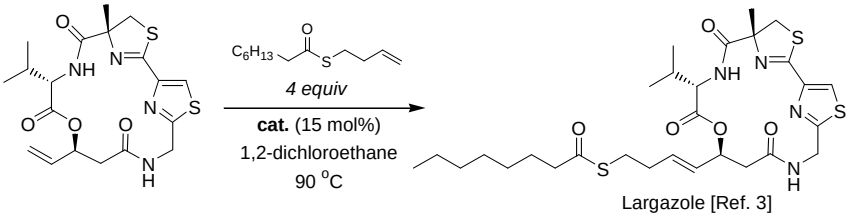
[1] Institute of Organic Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224, Warsaw, Poland

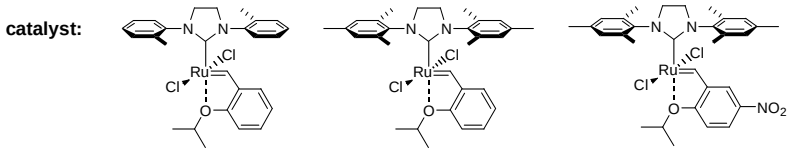
[2] Organometallic Synhesis Laboratory, Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093, Warsaw, Poland

Url: http://www.karolgrela.eu/

ABSTRACT

Ruthenium-catalyzed olefin metathesis reactions represent an attractive and powerful transformation for the formation of new carbon-carbon double bonds[1]. This area is now quite familiar to most chemists as numerous catalysts are available that enable a plethora of olefin metathesis reactions[2]. However, some transformations, such as formations of substituted double bonds, formations of strained rings, low-temperature metathesis, etc. still remain challenging[3]. This limitation can be solved by designing new more active catalysts[4] or searching for new reaction conditions[5].





During the lecture examples representative for both of the above mentioned strategies will be given [4-6].

REFERENCES

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[2] Thayer, A. Chemical & Engineering News 2007, 85 (07), 37.
[3] Seiser, T.; Kamena, F.; Cramer, N. Angew. Chem. Int. Ed. 2008, 47, 6483.
[4] Grela, K.; Harutyunyan; S., Michrowska, A. Angew. Chem. Int. Ed. 2002, 41, 4038.
[5] Kadyrov, R.; Bieniek, M.; Grela. K. DE Patent Application 102007018148.7, April 11, 2007.
[6] Samoj³owicz, C.; Bieniek, M.; Zarecki, A.; Kadyrov, R.; Grela, K. Chem. Commun. 2008,6282.

PL - 38

Plenary Lectures

Dr. P. T. Perumal

Scientist G and Head, Organic Chemistry Division, Central Leather Research Institute, Adyar Chennai- 20.

Basic research

i) Biocides based on Vilsmeier and Diels-Alder-adducts are available for valuation.
(ii) Process for the preparation of syntans having light resistance and filling characteristics have been developed at laboratory level.

Achievement

I am heading a team of more than 25 Scientific staff and Researchers in the Dept. of Organic Chemistry in CLRI. My work is mainly focused on (i)Synthesis of Heterocyclic compounds using Inverse Electron Demand Diels-Alder (IED) Strategy (ii) Synthesis of heterocyclic compounds by using Vilsmeier reagent (iii) Multi component reaction , Acylation , alkylation and oxidation reactions and (iv) Green chemistry approach to synthesis of heterocyclic compounds by Ionic liquid mediated reactions; Solvent free reactions; Microwave assisted reactions and Water mediated reactions: Most of the synthesised compounds were tested for their biological activities. This has brought out good number of publications in highly cited journals and also we have generated ECF to some extent.

Academic Qualifications

M.Sc.(Organic Chemistry)	First Class	Madurai University 1976
Ph.D (Organic Chemistry)		I.I. Sc., Bangalore 1981

Research Experience

35 years in the field of synthetic organic

Area of Specialization

Chemistry and medicinal Chemistry

Prestigious awards received

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

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Plenary Lectures

Application of catalysts in synthesis of heterocyclic compounds

P.T.Perumal
Scientist G, (Director Grade Scientist) & Head, Organic Chemistry Division, Central Leather Research Institute, Chennai-600 020

ABSTRACT

Catalysis is the process in which the rate of a chemical reaction is either increased or decreased by means of a chemical substance known as a catalyst. Unlike other reagents that participate in the chemical reaction, a catalyst is not consumed by the reaction itself. The catalyst may participate in multiple chemical transformations. Catalysts that speed the reaction are called positive catalysts. Catalysts that slow down the reaction are called negative catalysts or inhibitors. Substances that increase the activity of catalysts are called promoters and substances that deactivate catalysts are called catalytic poisons.

The chemical nature of catalysts is as diverse as catalysis itself, although some generalizations can be made. Proton acids are probably the most widely used catalysts, especially for the many reactions involving water, including hydrolysis and its reverse. Multifunctional solids often are catalytically active, e.g. zeolites, alumina and certain forms of graphitic carbon. Transition metals are often used to catalyse redox reactions (oxidation, hydrogenation). Many catalytic processes, especially those involving hydrogen, require platinum metals.

Heterogeneous catalysts are those which act in a different phases than the reactants. Most heterogeneous catalysts are solids that act on substrates in a liquid or gaseous reaction mixture. Homogeneous catalysts function in the same phase as the reactants, but the mechanistic principles invoked in heterogeneous catalysis are generally applicable. Typically homogeneous catalysts are dissolved in a solvent with the substrates.

We have used Lewis and Bronsted acids as a homogenous catalyst for the synthesis of novel heterocycles. The role of $InCl_3$, $AuCl_3$, AuCl, $FeCl_3$, $KHSO_4$, NH_2SO_3H as catalysts in Imino-Diels Alder reaction, Quinoline, Bis-indolylmethane synthesis, Oxidation, Cyclization, Baylis-Hillman reaction, and Multi-Component reactions were discussed in detail.

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Plenary Lectures

Prof. Virinder Parmar

Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi – 110 007, India
E-mail: virparmar@gmail.com

Professor Virinder Parmar, born on 2nd November 1948 at Allahabad (India), did B.Sc. Honours (1968), M.Sc. (1970) and Ph.D. (1978) from the University of Delhi. He has Postdoctoral / Visiting Scientist research experience of nearly ten years at Cornell University, Harvard University, University of Massachusetts Lowell, Polytechnic University and MIT (USA); University of Basel (Switzerland); Imperial College of Science, Technology and Medicine (London) and the University of Warwick (UK), and the University of Southern Denmark. He has been a faculty at the University of Delhi for the past 26 years, currently he is Full Professor of Chemistry at this University. He is a Visiting Full Professor at the Institute of Nanoscience Engineering and Technology, University of Massachusetts Lowell (USA) since March 2001. He has been appointed as Visiting Full Professor (Adjunct Professor) at the University of Southern Denmark for the period April 2008 – March 2013.

Professor Parmar's research interests include: Nanotechnology, Synthetic Organic Chemistry, Biocatalysis, Polymer Chemistry, Nucleic Acid Chemistry, Medicinal Chemistry, Green Chemistry, Advanced Materials and Chemistry of Natural Products. He has mentored 80 Ph. D. and Postdoctoral Associates, and has published three hundred and eighty three research papers (twenty more papers are under publication) in international journals of repute in addition to being co-inventor on eighteen US and Indian patents. He has organized 28 international conferences/symposia/seminars/workshops in the areas of his research interests.

He has handled thirty one research projects involving grants of nearly US Dollars 5.03 Million from various agencies in USA, UK, Germany, Denmark, Russia, France and India in international collaboration with twenty six research groups in USA, UK, Canada, Germany, France, Italy, Denmark, Belgium, Russia, India, Bulgaria and Czech Republic.

He has delivered Invited / Plenary Lectures at 122 International Conferences/ Symposia/Seminars/ Workshops and has lectured at 258 Institutions in twenty six Countries across the Globe. He has been on the Editorial Boards of several journals, to name a few – ChemSusChem, Mendeleev Communications, Indian Journal of Chemistry, Natural Products Communications, Arkivoc, Molecules & Biocatalysis and Biotransformation. He has been recognized with many awards and fellowships, most recent ones have been the Chemical Research Society of India (CRSI, Bangalore) medal, Professor ASR Anjaneyulu 60th Birthday Commemoration Award of the Indian Chemical Society (ICS, Calcutta) and Honorary Professorship at the University of Southern Denmark. He is a regular reviewer for several journals published by the American Chemical Society, the Royal Society of Chemistry (London), Elsevier Publications, etc., and is a member of the IUPAC Organic and Biomolecular Chemistry Division's Subcommittees on Biomolecular Chemistry and Green Chemistry.

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Plenary Lectures

Natural products-based (from *Piper & Tephrosia* species) anti-microbial, anti-inflammatory and antiplatelet agents

Virinder Parmar
Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi – 110 007, India
E-mail: virparmar@gmail.com

ABSTRACT

We have extensively worked on several plant species and isolated a large number of novel compounds belonging to different classes (alkaloids, polyphenols, steroids, amides, terpenoids, etc.).Many of them have shown interesting biological activities, remarkable of them has been our extensive work on polyphenol acetates leading to the discovery of a fundamental biochemical pathway involving acetyl CoA-independent enzymatic protein acetylation. Our seminal investigations have highlighted the unique biochemical and pharmacological action of polyphenol acetates. These act as the substrates for the well-known protein calreticulin and transfer acetyl groups to certain receptor enzymes, such as cytochrome P-450 linked mixed function oxidases (MFO), NADPH cytochrome c reductase, Nitric Oxide Synthase (NOS), protein kinase c (PKC) and glutathione S-transferase (GST) resulting in modulation of their catalytic activities. The purified enzyme from buffalo liver in the presence of 7,8-diacetoxy-4 methylcoumarin (DAMC) and several other polyphenol acetates was found to significantly enhance the NOS activity in human platelets and caused significant vasorelaxation. These polyphenol acetates and several natural products were also found to lower PKC levels and suppress the ICAM-1 and VCAM-1 expression, and were found to be good anti-inflammatory & anti-asthmatic agents.

Further studies have revealed that acetoxyphenols having the vicinal diacetoxy moiety are also good radical scavengers, thus enabling these compounds to block the formation of superoxide and other reactive oxygen species. Acetoxy polyphenols and several other classes of natural products were also found to be excellent inhibitors of chemical and radiation induced clastogenecity, and antifungal agents against various deadly lung fungal infections.

Details of these studies will be discussed in the presentation.

Financial support from DSIR (CSIR, Govt of India, New Delhi) and University of Delhi is acknowledged.

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Plenary Lectures

Prof.Dr. Johan Van der Eycken

Professor, Ghent University (Belgium), Laboratory for Organic and Bioorganic Synthesis, Department of Organic Chemistry, Krijgslaan 281 (S.4), B-9000 – GHENT (Belgium)
E-mail: Johan.Vandereycken@UGent.be

Johan Van der Eycken is Professor in Organic Chemistry and Head of the Laboratory for Organic and Bioorganic Synthesis (LOBOS) at Ghent Universtity (UGent), Belgium. He obtained his PhD degree in 1986 from Ghent University, Belgium, for research devoted to the total synthesis of podophyllotoxin and epipodophyllotoxin, lignans with antitumor properties, with Prof. Maurits Vandewalle as promoter. In 1986, he performed a postdoctoral stay with Prof. Manfred Schneider (Bergische Universität, Wuppertal, Germany) on the use of lipases in asymmetric synthesis. In 1987, he was appointed as a Lecturer at Ghent University, Belgium, where he was promoted to Assistant Professor in 1991. In 1992 he became Full Professor at the same university.

His main research topics are asymmetric synthesis mediated by transition metal catalysts (design and use of novel chiral ligands) and enzymes (lipase-catalyzed kinetic resolution), total synthesis of complex biologically active compounds (e.g. carba sugars, imino sugars, Lipid II analogues, macrocyclic antibiotics, e.g. Peloruside A), and solid phase synthesis of peptidomimetics and small organic molecules as privileged scaffolds for drug discovery.

PL - 40

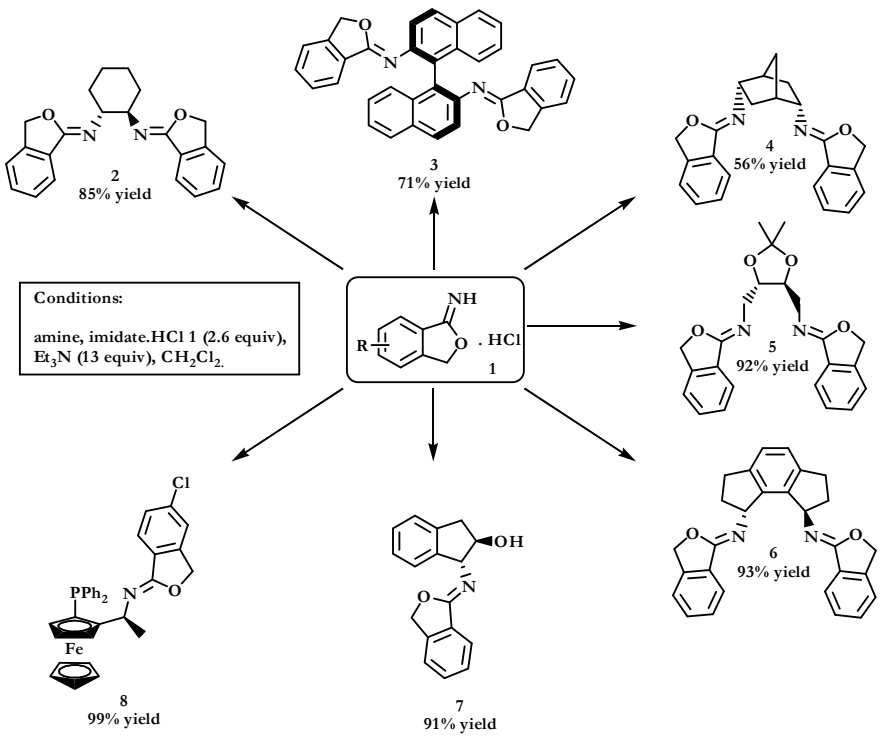
Plenary Lectures

A modular approach to chiral imidates: A new class of nitrogen-based chiral ligands

Johan Van der Eycken*, Timothy Noël, Katrien Bert, Koen Vandyck
Laboratory for Organic and Bioorganic Synthesis, Department of Organic Chemistry, Ghent University, Krijgslaan 281 (S.4), B-9000 Ghent, Belgium
E-mail: Johan.VanderEycken@UGent.be

ABSTRACT

Nitrogen-containing ligands are known as *cheap, readily accessible and stable* alternatives for phosphane ligands,[1] which are often very sensitive to air and require a multistep synthesis.[2] We wish to present a *combinatorial approach* to *a novel type of nitrogen-based mono- and bidentate ligands*.[3,4] These ligands are characterized by their *modular structure*, allowing an *easy one-step synthesis* by simply combining two readily variable precursors which are either commercially available, or can be reached in only a few steps: a cyclic imidate 1 and a (chiral) amine, respectively diamine. These ligands show *promising results* in e.g. the Cu(I)-catalyzed asymmetric aziridination of methyl cinnamate, in asymmetric diethylzinc additions to benzaldehydes, in the Pd(0)-catalyzed asymmetric allylic alkylation, and in asymmetric hydrogenations of alkenes.



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Plenary Lectures

Prof.Dong-Soo Shin

Professor, Department of Chemistry, Changwon National University, #9 Sarim-dong , Changwon, Kyongnam, 641-773, S. Korea
Tel: +82552133437; Fax : +82552133439, Cell: +821072771574
E-mail: dsshin@changwon.ac.kr

Experience

Professor	Mar. 1999 – Present
Associate Professor	Mar. 1994 – Feb. 1999
Assistant Professor	Mar. 1989 – Feb. 1994

Academic Honors

2001 The Pride Fellowship Awards Gyongnam Province, Korea

Education

Mar. 1974 – Feb. 1981	Bs. D.	Chemical Education, Department of Chemical Education, Gyeongsang National University, Jinju, S. Korea
Mar. 1981 – Feb. 1983	Ms. D.	Organic Chemistry, Department of Chemistry, Gyeongsang National University, Jinju, S. Korea
Mar. 1983. – Feb. 1987	Ph. D.	Synthetic Organic Chemistry, Department of Chemistry, Sungkyunkwan University, Seoul, S. Korea *Thesis*: "The Synthesis of Biologically Active Pheromones " Advisor: Prof. Suk-Ku Kang

Research Fellow

Department of Biochemistry, UT Southwestern Medical Center, Dallas, Texas (Professor John R. Falck's Lab.)

1. Visiting Professor Jan. 2001. - Feb. 2002.
2. Research Fellow June 1992. – Feb. 1993.
3. Post-Doctoral Fellow Mar, 1987. – Feb. 1989.

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Plenary Lectures

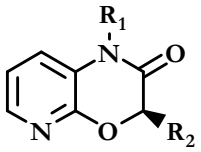
Efficient approach to the synthesis of novel heterocycles

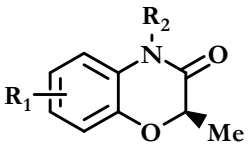
Dong-Soo Shin
Department of Chemistry, Changwon National University, #9 Sarim-dong , Changwon, Kyongnam, 641-773, S. Korea
E-mail: dsshin@changwon.ac.kr

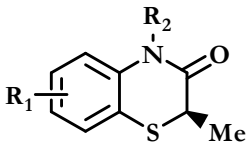
ABSTRACT

Novel optical *N*-substituted-2*H*-pyrido[*b*][1,4]oxazin-3(4*H*)-ones, *N*-substituted-2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-ones and *N*-substituted-2*H*-benzo[*b*][1,4]thiazin-3(4*H*)-ones with potential synthetic and pharmacological interest were designed and synthesized *via* Smiles rearrangement using different methods including conventional heating and microwave irradiation by one step and in one-pot synthesis. Investigation on reaction time, yield and purification procedure showed that the synthesis under microwave irradiation was much more efficient method to obtain *N*-substituted-2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-one, *N*-substituted-2*H*-benzo[*b*][1,4]thiazin -3(4*H*)-one and *N*-substituted-2*H*-pyrido[*b*][1,4]oxazin-3(4*H*)-one derivatives.

As second part, synthesis of (*R,R*)/(*S,S*)-2,2-dimethyl-2,7-dihydro-1*H*-oxireno[2,3-*c*]chromene and their derivatives will be presented. Potassium channels are exceptionally diverse both in variety and function. They play an important and complex role in the basic electrical and mechanical function of a wide variety of tissues, including smooth muscle, cardiac muscle and glands. With the aim of discovering new molecules with potassium channel activating properties, we have designed and synthesized derivatives of cromakalim, an important molecule which shows specific affinity towards potassium channels, based on the previous structure-activity investigation by applying different R4-and R6- substitutions.







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Plenary Lectures

Prof. Chung Man Chin

LAPDESF – Laboratory of Drug Design. Department of Drugs and Medicines - School of Pharmaceutical Sciences – University of Sao Paulo State – UNESP, Araraquara, SP, BRAZIL
E-mail: chungmc@fcfar.unesp.br

1983	Graduation in Pharmacy and Biochemistry, School of Pharmaceutical Sciences, University of Sao Paulo State, (FCF/UNESP), Brazil
1988	Msc in Pharmacology – Medicine Faculty. University of São Paulo, Ribeirão Preto, USP
1988	Teaching Assistant and Researcher in Medicinal Chemistry – FCF-UNESP, Brazil
1996	PhD in Pharmaceutical Sciences, Faculty of Pharmaceutical Sciences , USP, Brazil
1997	Doctor Professor in Medicinal Chemistry – FCF-Unesp, Brazil
2002 - 2004	Vice- head of Department of Drugs and Medicine – FCF-UNESP, Brazil
2002 - 2004	President of the Bioequivalence and Pharmaceutical Equivalence Committee –FCF-UNESP
2002	Member of the Pharmaceutical Sciences Post-graduation Committee –FCF-UNESP
2004 - 2008	Head of Department Drugs and Medicine – FCF-UNESP, Brazil
2004 - 2008	President of Araraquara Pharmaceutical Association- AFAR
2008	Vice –president of Araraquara Pharmaceutical Association- AFAR
1999	Coordinator of Course about Pharmacotherapy and Drug Interactions for professionals
2000	Graduate Doctor Professor- Course about *Prodrug design*
2004	Graduate Doctor Professor- Course about *Drug Interactions*
2006	Scientific Editor of the Journal *Revista de Ciências Farmacêuticas Básica e Aplicada*
2008	Scholarship in Research Productivity 2- CNPq

Member of the Medicinal Chemistry Division of SBQ – Brazilian Chemistry Society, "Ad hoc" advisor of Research and Graduation Funding Agencies: FAPESP, CNPq, FUNDUNESP, Ad hoc" advisor

Academic Advisory

13 master thesis concluded, 2 current
6 PhDs thesis concluded, 2 current
1 Postdoctorate supervision

PATENTS

US PATENT 2007/0072929A1 (approved 2009)
EUR – PATENT EP1685114B1 (approved 2008)
PCT/BR 2009/0409
PCT/ Br/000386- 2008
PI 0000220802234957/2008 (Br)
PI 018070081970/2007 (Br).
PI052097-2/2005 (Br)

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Plenary Lectures

TNF-alfa inhibitors potentially active against *Mycobacterium sp.*

SANTOS, J.L.[1]; YAMASAKI P.R.[1]; VIZIOLI, E.O.[1]; LEITE, C.Q.F.[2]; HIGUCHI C.T.[2], PLACERES, M.C.P.[3]; CARLOS, I.Z.[3] CHUNG, M.C.[1]

[1]Lapdesf – Laboratory of Prodrug design - Dept of drugs and medicines, [2] Dept of Biology Sciences, [3] Dept of Clinical Analysis, School of Pharmaceutical Sciences - University of São Paulo State - UNESP - Araraquara – São Paulo - Brazil

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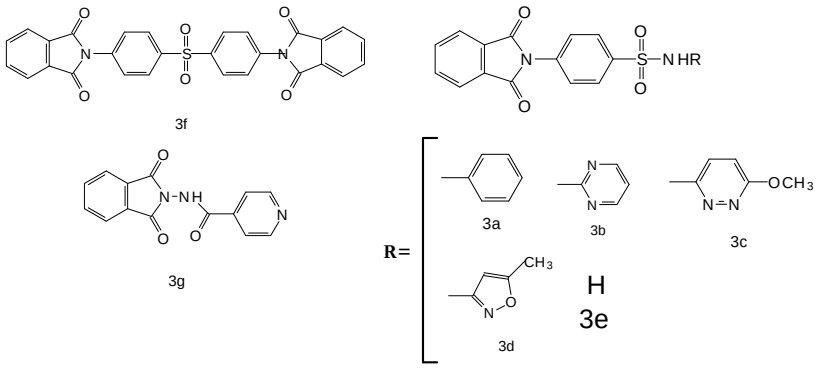
ABSTRACT

Mycobacterial infections, tuberculosis and leprosy, are an important cause of morbidity and mortality worldwide. Tumor necrosis factor-α (TNF-α), is a cytokine considered to be a primary mediator of the inflammatory response. Interventions that reduce the level of TNF-α have been associated with clinical benefit during active disease, particularly for leprosy patients undergoing acute immunopathological reactions, then the regulation of the level of TNF alpha production may be crucial in determining the outcome of mycobacterial infection. The purpose of this work is to synthesize and test antimicobacterial profile of new *N*-substituted phthalimides derivatives, structurally designed as hybrids of thalidomide and sulfonamides. The preparation of compounds 3a-e were obtained through the condensation of the phtalic anhydride with the corresponding sulfonilamides. The hybrid compound 3f has a double phtalimide substructure and 3g has a substructure of isoniazid. The anti-mycobacterial activity (MIC) -MABA technique- and the partition coefficient (log P) were determined: 62.5 μg/mL and 3.06; <3.9 μg/mL and 1.,63; 2.50 μg/mL and 2.63; 62.5 μg/mL and 2.28 for 3a, 3b, 3c and 3d respectively. The compounds 3e-3g had the partition coefficient (log P) determined as 1.40; 4.16 and 0.78. The results showed 3b as an active prototype against *Mycobacterium tuberculosis* and a candidate to molecular modifications. We observed that the more active compounds 3b and 3d showed the ability to increase nitric oxide in macrophage.



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Plenary Lectures

Prof. Athina Geronikaki

Aristotelian University of Thessaloniki, School of Pharmacy, Department Pharm.Chemistry, Thessaloniki, 54006, Greece
E-mail: Athina@chios.pharm.auth.gr; Geronik@pharm.auth.gr

WORK

1971-1978	Institute of Chemistry of Natural Products of Uzbek Academy of Science
1979-1980	Greek Company "Deras" as a chemical consultant, Greece
1980-1982	Factory of Phytochemicals "Diana" of Thessaloniki, (chemist)
1982	School of Pharmacy, Department of Pharmaceutical Chemistry of Aristotelian University of Thessaloniki
1998-2003	Asist. Professor
2003-2009	Assoc. Professor
2006-2010	Head of the laboratory
2009-2011	Vice-President of the School of Pharmacy

RESEARCH PROGRAMS

1. **1998 NATO project entitled:** "Organosilicon derivatives of thiazoles as potent prodrugs" collaboration with Prof. Zablocka (Latvia). (NATO Felloship)
2. **2002 NATO project entitled:** "Computer-assisted design and chemical synthesis of new biologically active compounds with required properties" collaboration with Dr. Lagounin (Institute RAMS) Russia (NATO Felloship)
3. **2004 NATO project entitled:** "Synthesis of acetylene derivatives of thiazoles". collaboration with Prof. Vasilevskii (Instituteof Chemical Kinetic and Combustion of Siberian Branch of Russian Academy of Science) (NATO Felloship).
4. **Coordinator of Europeanproject INTAS-00-0711, entitled:** "Computer-assisted combinatorial design, synthesis and testing of new cognition enhancers, anxiolytics and anticonvulsants". Countries-Participants: Greece, France, Portugal, England, Belgium, and 5 teams from Republic of Former Soviet Union (Moscow, Moldavia and Siberia).
5. Collaborative grant Greek-Russia , Moscow , 1999.
6. Collaborative grant Greece-Italy , Catania, 2000.
7. Grant from Italian government CNR, Parma, 2001.
8. National Project PITHAGORAS I.

AWARDNESS

2003 Silve medal from Scientific Partnership Foundation for the development of International Collaboration.
2010 Medal from Scientific Partnership Foundation for contribution in science

Participation in International Conferences 190

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Plenary Lectures

Synthesis of novel 3,4-diaryll-1,2,4-triazoles as well as 2-substituted thiazolo[4,5-*f*]isoquinolines/quinolines and benzo[1,2-*d*:4,3-*d'*]bisthiazoles as potent COX-1/2 inhibitors

N.I.Korotkih[1], N.V.Glinynaya[1], E.P.Pitta[2], K.S.Liaras[2], A.A.Geronikaki[2], M.Chakrabarty,[3] A.Mukherji[3]
[1]The L.M.Litvinenko Institute of Physical Organic & Coal Chemistry of the Ukrainian Academy of Sciences
[2]School of Pharmacy, Dep/t Pharm. Chemistry, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece
[3]Department of Chemistry, Bose Institute, 93/1, A. P. C. Road, Kolkata 700009, India
E-mail: geronik@pharm.auth.gr

ABSTRACT

A series of 3,4-diaryl-1,2,4-triazoles was synthesized by the ring transformation of the respective 2,5-diaryl-1,3,4-oxadiazoles with anilines including fluorine substituted ones in the presence of trifluoroacetic acid (TFA) in o-dichlorobenzene (o-DCB) at 180-200 °C in good yields (40-68 %) (scheme 1) according to method [1].

The composition and structures of new triazoles 2c-i were confirmed by the methods of elemental analysis, ^{1}H NMR spectroscopy and mass-spectrometry. In the ^{1}H NMR of triazoles 2a-i along with resonances of aromatic protons a characteristic signal of meso-proton (C^5H) is observed in the region of δ 8,9– 9,1 ppm in DMSO-d_6. The most acidic is meso-proton of compound 3b (δ 9,12 ppm). The indicated characteristics show that the acidity of azolic ring due to the presence of fluorine atoms is changed not much, and sometimes it is little perceptible. In the mass spectra of triazoles the molecular ions were obtained assigning the indicated structures.

On another hand, taking into account the importance of thiazole ring as a pharmacophore our interest was concentrated on the synthesis of annulated thiazoles as potent inhibitors of COX isoenzymes.

All the title compounds were evaluated for their COX inhibitory activity.

1 2a-i

Scheme 1

REFERENCES

[1] Korotkikh N. I., Kiselyov A. V., Knishevitsky A.V., Rayenko G. F., Pekhtereva T. M., Shvaika O. P. Chem. Heterocycl. Comp. (Latvia) 2005, 7, 1026

PL - 04

Plenary Lectures

Dr.Tushar Kanti Chakraborty

Director, Central Drug Research Institute, Chattar Manzil Palace, Post Box No. 173, Lucknow - 226 001, UP, India
Tel: 091-522-2623286, 2610932
Fax: 091-522-2623405 / 2623938 / 2629504
Email: director@cdri.res.in
http://www.cdriindia.org

Education

Ph.D. in 1984 from Indian Institute of Technology, Kanpur under the supervision of Prof.S. Chandrasekaran; Postdoctoral Fellow during 1984-87 at University of Pennsylvania,Philadelphia with Prof. K. C. Nicolaou.

Awards and Honors

- Shanti Swarup Bhatnagar prize for Chemical Sciences in 2002.
- Elected Fellows of the (i) Indian National Science Academy in 2007, (ii) Indian Academy of Sciences in 2003 and (iii) The National Academy of Sciences, India in 2000.
- NASI-Reliance Industries Platinum Jubilee Award in Physical Sciences in 2006.

Other Awards

(a) JC Bose Fellowship in 2008; (b) Ramanna Fellowship in 2007; (c) Andhra Pradesh Scientist Award in 2005; (d) Innocentive Champion in 2005; (e) Chemical Research Society of India Bronze Medal in 2002; (f) Dr. Basudev Banerjee Memorial Award of the Indian Chemical Society in 1999; (g) CSIR Young Scientist Award in 1991; (h) A. P. Akademi of Sciences Young Scientist Award in 1991.

Research Areas

Organic synthesis, peptides and peptidomimetics; designing new amide-linked molecular entities based on sugar amino acids and related compounds and studying their three-dimensional structures and properties.

Publications

Guided 22 PhD students and published over 150 papers in international journals with >2700 citations, H-index 29.

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Plenary Lectures

Dr.J.S.Yadav

Director,Indian Institute Of Chemical Technology, Hyderabad, INDIA

Dr. J. S. Yadav was born on 4th August, 1950 in Azamgarh District of Uttar Pradesh, INDIA. Dr. Yadav has obtained his masters in 1972 and doctorate in 1976 from India. He was a Post Doc at Rice University, Houston and UW, Madison in USA for 3½ years.

He returned to India and joined in CSIR service in 1981 at National Chemical Laboratory (NCL) Pune. Subsequently he moved to Indian Institute of Chemical Technology (IICT), Hyderabad in 1986. In 1989, he has been elevated as Head of the Department of Organic Chemistry Division (Natural products and synthetic organic chemistry), the largest research group at IICT.

Later in 2003, Dr. Yadav was appointed as director of the Indian Institute of Chemical Technology (IICT), Hyderabad, consisting of 1100 dedicated staff which includes 250 research scientists in R&D Divisions. He occupies **number 1** position among the top 21 scientists from India, short listed for their highest productivity in terms of publication **during the last 10 years**.

In a span of two and half decades of research career, Dr. Yadav has been able to successfully carry out extensive basic and applied research investigations in the synthesis of complex Natural products of biological relevance. He is specialist in asymmetric synthesis to create new chiral centers in complex organic molecules and utilize them effectively in synthesis of many bioactive molecules for example., Hydroxy fatty acid, Discodermalice, Rifamycin, Scytophycin, Calcimycin, Artemisin, Taxol etc. Dr Yadav's research group has successfully developed cost effective Technologies for special chemicals like Diltiazem, Ondaseyron, Pyrazinamide, Ketotifen, Mefloqauin, Tamoxifen etc., They have been very well received by the Indian and Overseas drug industries.The global majors like Smithkline Beecham (SB),Dupont, FMC and Ranbaxy, Lupin and Dabur have entered into medium term contract research agreement with his research teams. His research findings have been published in more than 726 research papers, patents and invited talks.

Dr Yadav's expertise and skills in organic chemistry are outstanding and is a member of prestigious scientific bodies like Department of Science and Technology, Technical Advisory Board (TAB) and a National representative of International Union for Pure and Applied Chemistry (IUPAC). He has received many academic and Industrial Awards viz., Shanti Swarup Bhatnagar Award (1991), Vasvik Award in Chemical Sciences & Technology (1999), Ranbaxy Research Award in Pharmaceutical Sciences (2000), Prof. Swaminathan 60th Birthday Commemoration Lecture Award (2002), Vigyan Ratna , Vigyan Gaurav Awards of Council for Science and Technology, Uttar Pradesh (2003)(2004), Goyal Award 2003, DOST Prof S K Sharma Medal and Chemcon Distinguished Speaker award 2006, CDRI oration award 2006, CHEMTECH award for Outstanding Achievement in R&D/ Innovation Institutions in Pharma + Biotech 2007, Laureate of the 22nd Khwarizmi International Award 2008, BHU Distinguished Alumnus Award. He is also a Fellow of JC Bose (DST, GOI) 2005, Third World Academy of Sciences for the developing World (FTWAS) 2006, Fellow of Indian Academy of Sciences (FASc) 2010, National Academy of Sciences (1993), Indian National Science Academy (1998), Member of A P Akademy of Sciences (2001) etc., He has to his credit over 885 research publications in various reputed national and International journals. He has also 20 International Patents and 27 Indian Patents to his credit. Dr Yadav is sought after as a research guide for doctoral and postdoctoral programs and more than **125 research scholars** obtained their degrees under his guidance. He is a recognized guide in most of the academic institutions in the country.

Dr Yadav is an eminent scientist with a high level of commitment to the cause of his profession viz., Natural Products-Organic Chemistry. He is married and blessed with two IITian sons

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Plenary Lectures

Dr.Michael N. Liebman

Managing Director, Strategic Medicine, Inc, Kennett Square, PA, USA 19348
E-mail: m.liebman@strategicmedicine.com

Michael N. Liebman, Ph.D. is the Managing Director of Strategic Medicine, Inc and also of Strategic Medicine, BV (the Hague, NL) after serving as the Executive Director of the Windber Research Institute since November, 2003. Previously, he was Director, Computational Biology and Biomedical Informatics at the University of Pennsylvania Cancer Center since September, 2000. He served as Global Head of Computational Genomics at Roche Pharmaceuticals and Director, Bioinformatics and Pharmacogenomics at Wyeth Pharmaceuticals. He was also Director of Genomics for Vysis, Inc and Director of Bioinformatics at the Amoco Technology Company. He is a co-founder of Prosanos, Inc (2000). He has served on the faculty of Mount Sinai School of Medicine in Pharmacology and Physiology/Biophysics. He serves on 14 international scientific advisory boards, consults for 5 pharma/biotech companies, the economic development programs in the Philadelphia Life Sciences Sector and the State of Illinois Biotechnology Commission and is on the Board of Directors of the Nathaniel Adamczyk Foundation for Pediatric ARDS. He has been a member of External Advisory Board of both the BRIN and INBRE programs in Delaware. He is an Invited Professor at the Shanghai Center for Bioinformatics Technology and is currently on the Human Health and Medicinal Chemistry Commission of the IUPAC. He received his PhD in protein crystallography and theoretical chemistry. His research focuses on computational models of disease progression stressing risk detection, disease process and pathway modeling and analysis of lifestyle interactions and causal biomarker discovery and focuses on moving bedside problems into the research laboratory to improve patient care and their quality of life. Recent activities also include computational approaches to drug safety and toxicology with specific emphasis on reducing animal testing.

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Plenary Lectures

Developing drugs for complex diseases: Understanding the clinical need

Michael N. Liebman
Managing Director, Strategic Medicine, Inc, Kennett Square, PA, USA 19348
E-mail: m.liebman@strategicmedicine.com

ABSTRACT

There exist two complementary but opposing approaches to drug design and development. The traditional (or bottom-up) approach attempts to identify molecular entities, natural or synthetic, which act on a specific target believed to be involved in the disease mechanism or process. This approach encompasses molecular screening, medicinal chemistry for modifying structure-activity relationships and computational chemistry and computational modeling including x-ray crystallography to study the active site interactions of the target macro-molecule.

We have been developing a top-down approach which starts in the clinic to better define and stratify the disease into sub-types based on disease progression and clinical presentation. This is intended to complement the stratification of patients based on their genetic and genomic make-up and improve the potential success for drug development beyond its current inefficient approach towards the realization of personalized medicine. The application of stratification approaches reduces the complexity of the disease space and improves the potential for identification of both uniquely specific and selective targets as well as impacts the business decisions critical within the pharmaceutical industry.

Applications of this approach, along with the impact on companion diagnostics, will be presented with a focus on breast cancer, herceptin and her2/neu testing.

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Plenary Lectures

Prof. Ravi Durvasula

Chief of Medicine, New Mexico VA Health Care System, Vice-Chairman of Medicine, Director of The Center for Global Health, Dept of Internal Medicine, University of New Mexico School of Medicine, Albuquerque, NM USA
E-mail: ravi.durvasula@va.gov

Postgraduate Training/ Work Experience

2005	New Mexico VA Health Care System, Albuquerque, NM Chief of Medicine, Albuquerque VA Medical Center
2005	University of New Mexico School of Medicine, Albuquerque, NM Associate Professor of Internal Medicine and Infectious Diseases; granted tenure in 2009
2005	University of New Mexico School of Medicine, Albuquerque, NM Director, Center for Global Health
2001- 05	Yale University Health Services, New Haven, CT Medical Director
2001- 05	Yale University School of Medicine, New Haven, CT Assistant Clinical Professor, Dept.of Epidemiology and Public Health
2000- 01	Yale University Health Services, New Haven, CT Chief of Clinical Resources Chief, Dept.of Laboratory Medicine
2000- 01	Yale University School of Medicine, New Haven, CT Associate Research Scientist and Lecturer, Dept. of Epidemiology and Public Health
1997-1999	Yale University School of Medicine, New Haven, CT Instructor, Dept.of Internal Medicine
1994-1997	Howard Hughes Medical Institute/ Yale University School of Medicine Howard Hughes Physician Postdoctoral Fellow
1993-1996	Yale University School of Medicine, New Haven, CT Fellow, Section of Infectious Diseases
1992-1993	Yale University School of Medicine, New Haven, CT Postgraduate Research Associate, Section of Infectious Diseases
1992	Baylor College of Medicine/ Methodist Hospital, Houston, TX Chief Medical Resident
1989-1992	Baylor College of Medicine, Houston, TX Resident, Department of Internal Medicine

PL - 46

Plenary Lectures

First and second generation paratransgenics: Tools for the control of global vector-borne diseases

Ravi V. Durvasula
Chief of Medicine, New Mexico VA Health Care System, Vice-Chairman of Medicine, Director of The Center for Global Health, Dept of Internal Medicine, University of New Mexico School of Medicine, Albuquerque, NM USA
E-mail: ravi.durvasula@va.gov

ABSTRACT

Despite great advances in public health worldwide, insect-transmitted infectious diseases remain a leading cause of morbidity and mortality. Additionally, the global impact of insect-transmitted diseases to agriculture exceeds $100 billion annually. Newly emerging patterns of certain vector-borne diseases such as malaria, West Nile encephalitis, tick-borne diseases and dengue fever underscore the impact of arthropod-borne illnesses.Currently, the best methods for control of many insect-borne diseases involve the use of chemical pesticides. Such campaigns may, in the short term, yield spectacular results. However, insecticide campaigns are hampered in several ways. Environmental toxicity and adverse effects on human health limit the use of many chemical pesticides. Emergence of insect resistance to a wide variety of insecticides has greatly undermined their efficacy. The cost of repeated applications of pesticides is often prohibitive. Therefore, the wholesale elimination of insect pests is neither practical nor probable. Evolving methods for control of vector-borne diseases rely on modification rather than elimination of insects. These strategies involve either direct transformation of an insect genome via mobile DNA elements (transgenesis) or expression of gene products in the host insect via transformed symbiotic or commensal microbes (paratransgenesis).

Paratransgenesis is a "Trojan Horse" approach to control of disease transmission. It employs the interactions between disease-transmitting vectors, bacterial commensals of the vectors and transmitted pathogens. Commensal bacteria are isolated and genetically transformed *in vitro* to export molecules that interfere with pathogen transmission. The genetically altered bacetria are then introduced into the host vector where expression of engineered molecules affects the host's ability to transmit the pathogen, i.e. its vector competence. This approach attempts to decrease pathogen transmission without adverse effects on vectors themselves. Furthermore, it employs, as a gene delivery mechanism, bacterial flora native to the host vector. There are several requirements for such an approach to work

1. A population of symbiotic or commensal bacteria must exist within a given disease-transmitting vector.
2. Arthropod-associated bacteria should be amenable to culture and genetic manipulation.
3. Genetically altered bacteria should remain stable.
4. Fitness of the genetically altered bacteria to re-infect host vectors should not be compromised.
5. Transgene products released from the genetically altered bacteria should interact with the target pathogen(s).
6. A method must exist for dispersal of the genetically altered bacteria amongst naturally occurring populations of vectors with minimal non-target spread of foreign genes to environmental bacteria and other arthropods.

Paratransgenic approaches are being developed for a spectrum of arthropod-borne diseases. The model system for paratransgenic control involves the vectorial transmission of Chagas disease, or American Trypanosomiasis, a disease with widespread prevalence in Central and South America. A new paratransgenic method is under development for control of sand fly-mediated leishmaniasis, with a focus on kalaazar endemic regions in Bihar, India. Modified paratransgenic systems are being explored for applications toward pathogens that cripple global mariculture. Finally, second generation paratransgenic systems are under development that will employ advanced nano-materials to achieve better targeting of recombinant molecules with minimal environmental impact of transgene release.

This session will provide an overview of activities in the Paratransgenesis Laboratory of The Centers for Cellular and Molecular Medicine and Global Health, Albuquerque, USA. This laboratory, under the direction of Dr. Ravi Durvasula, has played a leading role in development of paratransgenic applications. The current status of research in these systems will be reviewed.

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Plenary Lectures

Dr. K. P. Mohanakumar

Scientist G, Head, Division of Cell Biology & Physiology, Head, Project Monitoring & Evaluation Division, Indian Institute of Chemical Biology (CSIR, Govt. of India), 4, Raja S C Mullick Road, Kolkata
E-mail: mohankumar@iicb.res.in

Professional experience

He has been working solely in India, and has more than 30 years research experience in neuroscience research, with special reference to Parkinson's disease (PD). Joined as Scientist B in Indian Institute of Chemical Biology (IICB) in 1984, and initiated research on neurodegenerative diseases. Has established a strong neurodegenerative disease research laboratory, which is capable of handling several cellular & animal models of the disease.

Received short-term, advanced training at NIMH, NIH, Bethesda (1993 – in vivo brain microdialysis), at Universities of Essen (1998; path-clamp recording on primary cultures) and Goettingen (2000; path-clamp recording on brain slices), Germany, at Virginia Medical Center (2003 - PD cybrids production, 2006 - proteomics), Charlottesville, USA and at University of Kentucky (2010; Mass-spectrometry), Lexington, USA in varied areas of neurosciences.

Honours and Awards

- Elected Fellow - 2008 - National Academy of Sciences, India
- TWAS-ICSU-UNESCO Visiting Professor – 2004; 2005
- Raman Research Fellow – 2003, CSIR, Govt. of India
- National Bioscientist Award – 2000, DBT, Govt. of India
- ICMR Young Scientist Award -1992
- Indo-USAID S&T International Fellowship (1993)
- DBT Senior International Associateship (2006)
- ICMR International Fellowship (2010)
- Indo-Hungarian Delegation Member of INSA, 2003
- Indo-German Delegation Member of DBT, 2009
- Indo-US S&T Delegation Member, 2009
- Elected Member, Guha Research Conference, 2003
- Elected Fellow, Indian Academy of Neurosciences, 1999

Specific interests

Mitochondrial genes in PD and HD
Drug Discovery for PD and HD
Target evaluation for PD and HD

Scientific Society Awards

Uvnas Prize, Indian Pharmacological Society, 1999
Tulsabai Somani Education Trust Award, Indian Academy of Neurosciences, 1995

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Plenary Lectures

Ayurvedic medication for parkinson's disease: Two sides of a coin

Sengupta T[1], Vinayagam J[1], Nagashayana N[2], Gowda B[3], Jaisankar P[1] and Mohanakumar KP[1]*
[1]Indian Institute of Chemical Biology (CSIR, Govt of India), 4, Raja S.C. Mullick Road, Kolkata 700 032, India; [2]CGHS Dispensary # 3, Ministry of Health and Family Welfare (Govt. of India), Bangalore 560 004, India; [3]University of Agricultural Sciences, GKVK, Bangalore 560 065, India
E-mail: mohankumar@iicb.res.in

ABSTRACT

In the present study, we report the good and bad molecules present in the Indian traditional medicine. In the past we have conducted a prospective clinical trial on the effectiveness of *Ayurvedic* medication in a population of Parkinson's disease (PD) patients. A single dose of a concoction in warm milk of the herbs *Mucuna pruriens*, *Withania somnifera*, *Hyoscymus reticulata* and *Sida cordifolia* contained an average of 200 mg dose of L-DOPA. Therefore the benefits derived from the *Ayurvedic* medication was attributed to the content of dopamine precursor present in the preparation[1]. Later studies revealed better benefits with *M. pruriens* alone, which contained the major portions of L-DOPA, compared to pure L-DOPA in a clinical trial and in a study conducted on PD animals.

In a national program of research on traditional medicines in India, we have adapted strategies to segregate molecules from each of these plant extracts, and then carefully removed L-DOPA contained therein, and tested each of these sub-fractions and the predicted/isolated and synthesized molecules for any anti-PD activity in 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP), rotenone and 6-hydroxydopamine (6-OHDA)-induced parkinsonian/hemiparkinsonian animal models. The herbs were collected by a registered Govt. *Ayurveda* practitioner, and formed part of the lots procured for PD patients' use. These samples were further authenticated by the agriculturist. The samples were processed by the chemists and the chemical prints and bioassays for the studies were conducted jointly by biologists and the chemists. We report here two classes of molecules contained in these plants, one of which possessed severe pro-parkinsonian (phenolic amine derivatives) and the other having excellent anti-parkinsonian potential (substituted tetrahydroisoquinoline derivatives) [2]. The former has been shown to cause severe dopamine depletion in the striatum of rodents, when administered acutely or chronically. It also caused significant behavioral aberrations, leading to anxiety and depression [3]. The latter class of molecules administered in animals made parkinsonian following subacute administration of MPTP, caused reversal of behavioral dysfunctions and significant attenuation of striatal dopamine loss. These effects were comparable or better than the effects of the anti-parkinsonian drug, selegiline. These effects of the molecule were reproducible in rotenone and 6-OHDA hemiparkinsonian models of PD in rats.

Although there existed significant medical benefits that could be derived to patients due to the synergistic actions of several molecules present in a traditional preparation, accumulated data in our laboratory suggest complicated mechanisms of actions of *Ayurvedic* medication. Our results also provide great hope for extracting, synthesizing and optimizing the activity of anti-parkinsonian molecules present in traditional *Ayurvedic* herbs, and for designing novel drugs with novel mechanisms of action from the Indian traditional system of medicine, *Ayurveda*.

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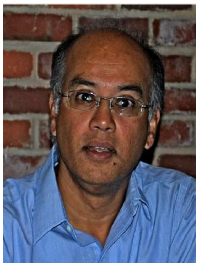
Plenary Lectures



Dr. Kollol Pal

CEO, Mnemosyne Pharmaceuticals Inc, USA

Dr. Kollol Pal is an organic chemist by training and brings 25 years of research and management experience in both pharmaceutical and biotech companies. He is the founding CEO of Mnemosyne Pharmaceuticals, a start-up company in Providence, RI, that is developing a novel research platform called Subunit Selective NMDA Receptor Modulators, SNRMs, that targets small molecule therapeutics for neuropsychiatric diseases including schizophrenia and Alzheimer's disease. Previously he has been the founding CEO of two start-up ventures (Satori Pharmaceuticals and Rishi Pharmaceuticals), and has had scientific leadership roles in a number of other biotech companies including Mitotix (acquired by GPC Biotech) and Neogenesis (acquired by Schering Plough). He began his research career at BoehringerIngelheim Pharmaceuticals where he was involved in the development of Nevirapine®, the first non-nucleoside reverse transcriptase inhibitor for HIV-AIDS. He received his undergraduate training in chemistry at Cornell University. Dr. Pal obtained his Ph.D. in organic chemistry at the Massachusetts Institute of Technology and carried out post-doctoral research at the Johns Hopkins University. Dr. Pal also obtained his MBA at the Sloan School of Management at MIT.

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Plenary Lectures

Ajulemic acid: A novel CB1/2 agonist for neuropathic pain

Kollol Pal
CEO, Mnemosyne Pharmaceuticals Inc, USA

ABSTRACT

Ajulemic Acid is a novel selective CB1/2 receptor agonist that is currently in clinical development for neuropathic pain. Ajulemic Acid is structurally related to the well-known cannabinoid, THC, however, it does not have any of the psychotropic side effects generally associated with the cannabinoids. Ajulemic Acid has been in over fifteen animal models of pain and inflammation and has demonstrated clinical efficacy in refractory neuropathic pain. The biological and clinical results of this novel cannabinoid derivative will be presented.

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Plenary Lectures

Dr. Jennifer S. Laurence

Associate Professor, Pharmaceutical Chemistry, University of Kansas, USA

Jennifer S. Laurence was recently tenured and promoted to Associate Professor of Pharmaceutical Chemistry at the University of Kansas. She received her PhD in Chemistry from Purdue University under the advisement of Dr. Patricia LiWang and conducted postdoctoral research in Structural Biology in the laboratory of Dr. Cynthia Stauffacher at Purdue. She is an expert in recombinant protein production, purification of proteins from cellular sources, and in defining the relationship between a protein's structure and stability, using biophysical tools and high-resolution solution NMR. Her recent work on understanding the mechanisms by which proteins degrade physically has been published in *Biochemistry*, *Journal of Pharmaceutical Sciences* and *Molecular Pharmaceutics*. Research in her laboratory has resulted in two patent applications, one involving a novel metal-binding tripeptide tag and the other a tag-based method for affinity purification and stabilization of proteins expressed using mammalian cell culture. Dr. Laurence is a member of the American Chemical Society (ACS). She serves on the ACS Committee on Science and has chaired sessions at National Meetings on Follow-on Biologics: Analytical methods of comparability and Biophysical and Biomolecular Symposium: Protein Stability and Interactions and Analytical Methods. She also serves on the Editorial Advisory Board of Journal of Pharmaceutical Sciences.

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Plenary Lectures

Identifying residue-specific contributions to protein stability and stabilization

Jennifer S. Laurence
Associate Professor, Pharmaceutical Chemistry, University of Kansas, USA

ABSTRACT

The number of proteins being developed as therapeutics has risen dramatically because of their tremendous specificity, which limits side effects. Unfortunately, these fragile molecules are prone to inactivation by unfolding and aggregation. It is commonly reported that the thermal stability of a protein depends on its structure, but it is also evident that the solution environment in which a protein resides affects its structural integrity and aggregation behavior. Many techniques exist that can monitor the outcome that changing solution conditions has on a protein's structural stability, but little information is available to explain how or why these changes in solution composition alter stability. We have undertaken a study using high-resolution solution NMR to explore the mechanisms by which a protein is affected by its environment. Two-dimensional NMR was used to monitor changes in individual residues within proteins during titrations. The data indicate that specific sites within a protein are perturbed by a change in solution conditions and unique types of perturbations induce changes at different sites within the protein. Interestingly, sites with closely related sequences and analogous structures did not respond similarly, suggesting that local packing among side chains may strongly influence protein stability.

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Plenary Lectures

Prof.Jochen Lehmann

Chairholder of Pharmaceutical/Medicinal Chemistry, Institute of Pharmacy, Former Dean of the Faculty of Biology and Pharmacy, Friedrich-Schiller-University of Jena, Philosophenweg 14, 07743 Jena, Germany
Tel: + 49 - 3641 - 949803; Fax: + 49 - 3641 - 949802
E-mail: j.lehmann@uni-jena.de

Research Interests

The group is of Medicinal Chemistry orientation

- Discovering small molecules as agents for the prevention and treatment of Alzheimers and other neurodegenerative diseases.
- Design, synthesis and screening of novel dopamine and serotonine receptor ligands as potential neuroleptics
- Nitric oxide releasing substances

Education

1964	Abitur (finishing High School) in Düsseldorf, Germany
1964-1970	Study of Chemistry, University of Bonn, Diploma
Juli 1972	Promotion to Dr. rer. nat. (excellent) Institute of Organic Chemistry, University of Bonn.
1972-1973	Post-doc-fellowship (German Research Foundation), Institute of Organic Chemistry, University of Bonn.
1973-1976	Study of Pharmacy.
1980	Habilitation for Pharmaceutical Chemistry, Institute of Pharmacy, University of Bonn

Profession

1983-1984	Professor (C2) for Pharmaceutical Chemistry, University of Bonn
1985-1990	Professor (C2) for Pharmaceutical Chemistry, University of Hamburg
1990-1999	Professor (C3) for Pharmaceutical Chemistry, University of Bonn.
1999-2000	Professur (C4) for Pharmaceutical Chemistry, University of Bonn.
2002-2010	Professor (C4) and Chairholder for Pharmaceutical/Medicinal Chemistry, University of Jena.
From 2010	Visiting Professor at King SaudUniversity Riyadh, Saudi Arabia
1998-1999	Head of the Institute of Pharmacy, University of Bonn.
1998-2002	Head of the German Pharmaceutical Society for Northrhine-Westfalia.
2002-2005	Head of the Institute of Pharmacy, University of Jena,.
2005-2009	Dean of the Faculty of Biology and Pharmacy, University of Jena.
From 2005	Member of the Senat of the University Jena.

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Plenary Lectures

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Plenary Lectures

Dr. S. B. Katti

Scientist G, Medicinal Chemistry Division, Central Drug Research Institute, Lucknow
Tel: 0522-2212411-18 PABX Ext. 4447, 4373 (O), 0522- 2788912 (R)
E-mail: sb_katti@cdri.res.in

Academic qualification

B.Pharm.	Bangalore University, Bangalore,	1972
M.Pharm.	University of Mysore, Mysore,	1975
Ph.D.	University of Mysore, Mysore,	1980

Positions held

1981-82 Postdoctoral Fellow, University of Zurich, Zurich, Switzerland.
1982-86 Research Associate, University of Chicago, Chicago, U.S.A.
1986 onwards Scientist, Central Drug Research Institute, Lucknow.

Fields of specialization

Medicinal Chemistry and Bioorganic Chemistry

Areas of interest

Chemistry of Nucleic Acids, Peptides and Protein-DNA Interactions.

Number of Publications

More than **75** in peer reviewed journals

Patents

IndianSeven
US patentTwo
EU patentTwo
US patent application accepted

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Plenary Lectures

Design and synthesis of thiazolidine-4-ones new antihyperglycaemic agents

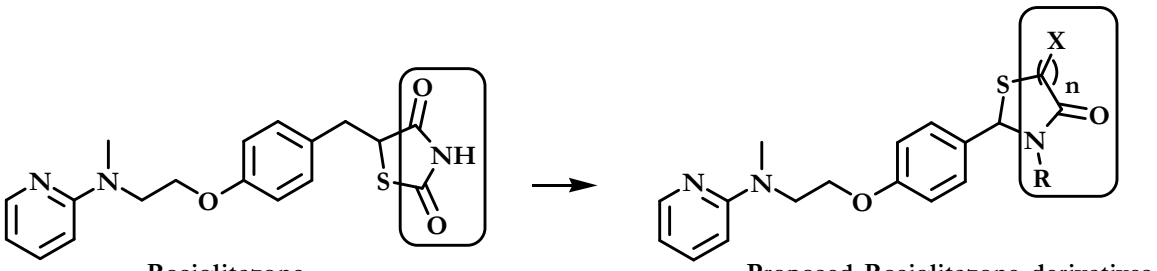
S. B. Katti
Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow.
E-mail: sb_katti@cdri.res.in

ABSTRACT

One of the important developments in type 2 diabetes therapy has been the introduction of thiazolidinediones (TZDs); a class of antihyperglycaemic agents that enhance insulin sensitivity through activation of Peroxisome Proliferator-Activated Receptor (PPAR-γ), a nuclear receptor involved in glucose homeostasis and adipogenesis. The drugs from this class, pioglitazone and rosiglitazone are currently being used worldwide for the treatment of type 2 diabetes.

The basic structure of a TZD comprises of an acidic head group, a central phenyl ring and a hydrophobic tail group joined by alkyl linkers. Since their discovery a lot of SAR-studies have been carried out with extensive modifications at the head and tail segments to obtain molecules with better therapeutic profile. A few compounds have displayed interesting antihyperglycaemic activity suggesting that modifications at either site could modulate the biological activity. Compounds like balaglitazone, which has successfully completed phase III clinical trials and rivoglitazone, which is currently in phase III clinical trials are two such compounds which display better pharmacological profile than the existing TZD drugs.

Encouraged by these findings during the present study a series of head group modified analogues having thiazolidine-4-one as a head group (figure 1) keeping rosiglitazone side chain as a template were investigated. Design, synthesis and biological activities of the new derivatives will be presented.



Rosiglitazone **Proposed Rosiglitazone derivatives**

Figure 1 : R = H, alkyl, aryl etc; X = H, -CH_3; n = 1, 2

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Plenary Lectures

Dr. Hariprasad Vankayalapati

Chief Scientist, Medicinal Chemistry, Huntsman Cancer Institute,
Salt Lake City, UT 84112, USA

Dr. Hariprasad is currently working for the Huntsman Cancer Institute's Center for Investigational Therapeutics division as a Chief Scientist overseeing the Medicinal/Computational Chemistry programs. Prior to this position Hariprasad was working for SuperGen Inc., as a Chief Scientist/ Director of Medicinal Chemistry from 2006-2009. Currently he is consulting and serving as advisor for SuperGen. He also served as Director of Medicinal Chemistry and co-founding member of startup Montigen Pharmaceuticals started in year 2003. Hariprasad was a key player both at the SuperGen/ Montigen company's Medicinal, Organic and Computational chemistry capabilities and he lead the expansion of in-house novel chemical entity libraries and established new strategic drug discovery programs in Oncology, inflammation and infectious diseases. This has led to the discovery and development of 2 clinical candidates currently in Phase I and Phase IB human clinical trials, 2 candidates in IND enabling studies and 4 candidates in the pre-clinical pipeline.

Hariprasad had previously served as Director of Chemistry at Neuropro Technologies Inc. Prior to his appointment at Neuropro; he was an Associate research scientist and senior postdoctoral fellow in Medicinal Chemistry division at the Arizona Cancer Center of the University of Arizona. From 1998 to 2000 he was a postdoctoral researcher in Organic Chemistry at the University of Sunderland, England and also worked for Ranbaxy Research Laboratories, New Delhi in India as a research scientist on infectious and CV drug discovery programs. Hariprasad received his Ph.D. in Medicinal Chemistry from the Institute of Chemical Technology (formally, UDCT) of the University of Bombay in 1996 and M. Pharm in Pharmaceuticals Chemistry from KLEs College of Pharmacy, JNMC Belgaum. He is the author of over 49 research publications related to the Organic, Medicinal and Computational Chemistry and holds five granted and 19 PCT/US/IN published patents.

His research interests includes; rational design and synthesis of small molecule therapeutics targeting cell signaling pathways particularly protein kianses, proteases, GPCR, PPI, transcription factors and cell-surface proteins. He is actively collaborating on several projects both at industry and institution level for the discovery and development of agents for treating cancer, inflammatory/metabolic and infectious diseases.

Invited Lectures

Prof.Anamik Shah

Department of Chemistry,Saurashtra University, University Road,Rajkot – 360 005, Gujarat (INDIA)
E-mail: anamik_shah@hotmail.com

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.

Ph.D. Refereeship

Dr. Anamik Shah is currently holding Ph.D. Refereeship in more than 20 Universities in India and abroad.

Collaborations (International)

1 Meiji Pharmaceutical University, Tokyo, Japan
2 Institute de Science, Pharmacology, University of Siena
3 Institute of Microbiology, Albert Szent George Medical University, Szeged, Hungary
4 Faculty of pharmaceutical science, Josai University, Saitama, Japan
5 Katholik University, Leuven, Belgium
6 Institute of Biomedical Sciences, Acedemia Sinica, Taiwan
7 Vienna University of Technology, Vienna (Austria)
8 National Institutes of Health, USA

Collaborations (National)

1 Dabur Research Foundation, Gaziabad
2 Nicholas Piramal Research Center, Mumbai
3 Defence Institute of Physiology & Allied Sciences, University of Mysore, Mysore
4 Alembic Limited, Vadodara
5 Claris Life Sciences, Ahmedabad

Country visited for scientific purpose

The Netherlands, Germany, France, Italy, Switzerland, Greece, United Kingdom and United State of America.

Research Projects

1. Several Research Project of worth ` 7 to 8 crores handled, completed and ongoing with various agencies like Department of Science and Technology (DST), New Delhi, NIH USA, Department of Atomic Energy (DAE)-BRNS, University Grant Commission (UGC), New Delhi, National Medicinal Plant Board, New Delhi and MSME Foundation, supported by DST Program. Projects completed successfully with leading Pharmaceuticals industries like Alembic Limited, Astrazeneca USA, Claris Life Sciences ltd, Dabur Research Foundation and Piramal Life Science.
2. NIH-USA funded "Structure-Based Development of Non-neucleoside anti-HIV-1 RT Drugs. With Prof. Virendra N. Pandey, NJ, USA & Dr. Tanaji Telele, NY, USA.

Invited Lectures

Discovery of NCE's at Saurashtra University

Anamik Shah
Department of Chemistry,Saurashtra University, University Road,Rajkot – 360 005, Gujarat (INDIA)
E-mail: anamik_shah@hotmail.com

ABSTRACT

Drug discove ry is a tedious and extremely expensive affair. Besides huge advancement in analytical technology, instrumentation and increased safety parameters for human beings, New Drug Discovery process is an extremely slow and mutibilinear affair. Pharmaceutical industry in 21st century saw significant growth in terms of discovery and development of number of therapeutic agents. At Department of Chemistry, Saurashtra University, Rajkot, we are continuously engaged in drug discovery process since past 2-3 decades. As an outcome, we have discovered some NCE's namely NM-140, DP-7, KUQ-18 etc that showed promising activity for the treatment of Tuberculosis, Multi Drug Resistant (MDR) Modifiers for cancer chemotherapy and Inflammation. Additionally, Department has set an ideal example in transfer of the technology from laboratory to Pharma Industries. The presentation will highlight the further details and advancement, challenges and other opportunities which may play significant role in discovery of novel therapeutic agents will be highlighted.

Invited Lectures

Prof.N.C.Desai

Medicinal Chemistry Division, DST-FIST Sponsored Department,Bhavnagar University, Bhavnagar-364 002, India
Email: dnisheeth@rediffmail.com

Area of Specialization

Organic and Medicinal Chemistry, Intellectual Property Rights & Management, Entrepreneurship in Academic Institutes

Academic Qualifications

M Sc. Ph.D.

Research Experience & Training

27 Years research experience

Publications

50 Research papers in reputed journals. Delivered an invited talk in the national and international conferences and chaired the several sessions.

Ph. D. Guidance

Twenty six students have obtained Ph. D. degree and Nine students are working for their Ph. D. Degree

Distinguished Awards

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

Invited Lectures

4-Oxo-thiazolidines: Important scaffolds in the new millennium for the development in pharmaceutical industries

N C Desai,
Medicinal Chemistry Division, DST-FIST Sponsored Department,
Bhavnagar University, Bhavnagar-364 002, India
Email: dnisheeth@rediffmail.com

ABSTRACT

The potential of 4-oxo-thiazolidines (TZDs) (2,4-thiazolidinediones, 2-thioxo(imino)-4-thiazolidones) as drugs is under consideration medicinal chemistry since the beginning of the 20th century.[1] Currently, 4-thiazolidones are considered as a new class of antidiabetic (insulin-sensitising) drugs and potent aldose reductase inhibitors, which possess potential for the treatment of diabetes complications (cataract, nephropathy, neuropathy).[2] Novel 4- thiazolidones are undergoing different stages of clinical trials as potential thyromimetic, antimicrobial, antiviral, anti-ischaermic, cardiovascular and anticancer drugs. A row of 5-arylidene-4-thiazolidones (phospholipase A2 inhibitors and dual COX- 2/5-LOX inhibitors) is under clinical trials as potential anti-inflammatory drugs.[1] Some original 4-thiazolidones are undergoing different stages of clinical trials as potential thyromimetic,[3] antimicrobial,[4] anti-HIV,[5] cardiovascular[6] and anti-cancer[7] drugs. In recent years, several new methods for the preparation of thiazolidinone derivatives and reactions have been reported in the literature.

The biological significance of this class of compounds impelled us to synthesize the new 4-thiazolidinone and 5-arylidene derivatives having different pharmacological properties. Our research group has focused on the synthesis and biological profile of the 4- TZDs. We have screened our novel class of 4- TZDs and 5-arylidene derivatives as anti-HIV,[8] anti-cancer,[8] anti-tubercular,[9] antibacterial,[10] antifungal[11] and anticonvulsant[12] agents. On the basis of the results received as part of random screening, we may conclude that 4- TZDs is an important scaffold for future drugs.

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[6] P C Stafylas, P A Sarafidis and A N Lasaridis, International J of Cardiology 131, 2009, 298.
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[11] N C Desai, A M Bhavsar, A Kumar, Chemistry An Indian Journal 3, 2006, 140.
[12] N C Desai, M R Shiradkar and K C Akula, Arkivoc xiv, 2007, 1.

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Plenary Lectures

Design strategies targeting type II and allosteric sites: New trends and opportunities beyond type I kinase domain site

Hariprasad Vankayalapati
Chief Scientist, Medicinal Chemistry, Huntsman Cancer Institute,
Salt Lake City, UT 84112, USA

ABSTRACT

Most of the protein kinase inhibitors currently in discovery phase, clinical stage development and or approved so far are ATP competitive Type I inhibitors which are associated with lack of specificity for individual kinases. This is due to high degree of conserved sequences of ATP-binding pocket within the family of kinome. Recent structural information have revealed that targeting non-ATP binding sites such as Type II and or Allosteric inhibition sites may offer a promising strategy for designing inhibitors in order to address the selectivity. The fragment or scaffold-based design approaches together with virtual ligand screening methods and our success in finding specific Type II and Allosteric inhibitors will be discussed in this presentation.

Invited Lectures

Prof.Sartaj Tabassum

Professor, Department of Chemistry, Aligarh Muslim University, Aligarh-202002, India
E-mail: tsartaj62@yahoo.com

Research Awards

2004-2005 Biotechnology Overseas Associateship Award
(Ministry of Science and Technology, Department of Biotechnology, Govt of India) JRF, SRF, RA CSIR, New Delhi

Academic Record

Country visited: USA, China, Italy

National and International Collaborations

- School of Life Sciences, University of Science and Technology, Hefei, China
- Department of Chemistry, University of Camerino, Italy.
- National Institute of Immunology, Aruna Asaf Ali Marg, New Delhi.
- ACTREC Tata Memorial Cancer Research Center, Mumbai.
- Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai.

Major Research Projects Completed

UGC, CSIR, DBT, TWAS

Membership in Professional bodies

Chemical Research Society of India (CRSI) (Life member)
Indian Council of Chemists (ICC) (life member)
Indian Society of Chemists and Biologists (ISCB)(life member)

Research Areas

- Bioinorganic Chemistry
- Molecular Drug Design, Isolation and their anticancer activity via Gene Mediated

Administrative Experience

Provost S.S. Hall (North)AMU,Aligarh 14th Mach 2007- 20th June 2009

Member

→ Member Academic Council, AMU,Aligarh Sep.2007- 20th June 2009
→ Member AMU Court, Sep. 2007- 20th June 2009

Invited Lectures

Metallic saviour : Chemical and biotechnological developments of metal based macro to nano chemotherapeutics

Sartaj Tabassum
Department of Chemistry, Aligarh Muslim university Aligarh -202002, India
E-mail: tsartaj62@yahoo.com

ABSTRACT

In the field of medicinal chemistry, inorganic materials are gaining attention owing to their diverse molecular and unique spectral features. Recent literature reveals that the metal based inorganic architecture display versatile utility from synthetic scaffolds for the preparation of small molecular therapeutics , to gene delivery vector in the field of molecular biotechnology . Since pharmacological target of the most metal-based cancer chemotherapeutics is cellular DNA and N7 atom of purines located in the major grooves of double helix are the most accessible and reactive nucleophilic sites for binding to DNA , interaction of metal complexes with DNA is of paramount relevance . Targeting DNA at the molecular level with specificity will lead to more effacacious therapeutics .Ligands can modify the reactivity, lipophilicity, oral/systematic bioavailability of metal ions, stabilization of oxidation state and substitutional inertness depending on the requirements for chemotherapy . In this regard, the rapidly expanding field of glycobiology has a positive impact on medicinal inorganic chemistry .Furthermore, potential benefit of carbohydrate,pyrazoles and peptides appended metal complex lies in the modulation of hydrophilicity or lipophilicity which not only affect the cellular uptake of the compounds but also helps in their facile transport at the molecular level.The size of the drug molecules macro to nano alters the dose and regulates the cellular uptake by the drug. Despite the development of numerous compounds that bind and inhibit the molecular target selectively, their localized delivery is a major discrepancy in effective clinical treatment. The nanotherapeutic approach has been introduced for the effective administration of anticancer drugs to the desired target with no collateral damage to the healthy tissues. Nanoparticles being smaller than the cancer cells can easily pass through cell barriers which could afford proper biodistribution, prolonged circulation time and reduced systemic toxicity.

Invited Lectures

Dr. Raj Rajur

Chairman & CEO, **CreaGen Biosciences, Inc., Woburn, MA, USA**

Dr. Rajur holds a PhD degree in synthetic organic/Medicinal chemistry and has enjoyed a distinguished career in the academic community and the pharmaceutical industry with a broad range of experience in medicinal chemistry and drug discovery. He has authored more than 30 papers in peer-reviewed journals and holds three US patents.

Dr. Rajur's academic career includes appointments at the Southwestern Medical Center in Dallas, Center for Engineering in Medicine and Biology at Massachusetts General Hospital and Harvard Medical School. Boston College and Northeastern University. In the industrial sector, he has held scientific and managerial positions at ArQule and Millipore Corporations. Currently he serves as Chairman and CEO of a biotechnology company, CreaGen Biosciences, Inc. in Woburn, MA USA,

Dr. Rajur, also, serves as the reviewer for the Journal of Pharmaceutical Sciences and presently is the Program Chair for the Medicinal Chemistry Division of the Northeastern Section of the American Chemical Society.

Dr. Rajur's expertise is with small molecule drug discovery, specifically targeted towards Diabetes, cancer and anti-infective therapeutics and the development of prodrug pharmaceuticals.

Invited Lectures

Collaborative drug discovery efforts to overcome the gap between chemistry and biology

Raj Rajur
CreaGen Biosciences, Inc, 23 Rainin Road, Woburn, MA 01810 USA
E-mail: rrajur@creagenbio.com

ABSTRACT

Collaborative research is one of the ways to bridge the gap between the chemistry and biology spectrum by involving scientists from varied background to understand and find a better solution to discover bio-active molecules. CreaGen Biosciences is involved in such efforts with many academic and biotechnology companies. I will discuss few case studies wherein opportunities and challenges with this approach have shown greater promise to find clinical candidates cost-effectively in a rapid fashion.

Invited Lectures

Prof. George O'Doherty

Northeastern University

Dr. O'Doherty is a native of Ireland, he grew up in Greenfield, Indiana as the child of two organic chemists. Having decided at a young age to go into the family business, he attended Rensselaer Polytechnic Institute where he did undergraduate research with Prof. Alan R. Cutler and in 1987 he received his BS. Later that year, he moved to The Ohio State University and began to work towards his Ph.D. in the labs of Leo A. Paquette. After receiving his Ph.D. in 1993, he joined the labs of Prof. Barry M. Trost at Stanford University and worked as an NSF postdoctoral fellow. In 1995 he moved to Imperial College, London and spent a year working as a postdoctoral fellow in the labs of Anthony G. M. Barrett. Dr. O'Doherty began his academic career back in the states where he started a research program interested in the use of asymmetric catalysis for the synthesis of biologically important natural products and carbohydrates. After six and eight year stays at the University of Minnesota and West Virginia University he moved to Northeastern University in Boston where in 2010 he was promoted to Professor of Chemistry.

Invited Lectures

The de novo synthesis of biologically important natural products and carbohydrate chemistry with application to medicinal chemistry

George A. O'Doherty
Northeastern University

ABSTRACT

My research group has been working in two related areas of organic synthesis: carbohydrate synthesis and natural product synthesis. The unifying theme that connects our research in these two areas is our use of asymmetric catalysis. Fundamental to our approach is the development of highly efficient routes that transform, via catalysis, inexpensive achiral starting materials into enantiopure products, which are poised for the conversion into complex molecules with biologically relevant properties (i.e. enantioselective synthesis of a new "chiral pool" via asymmetric catalysis). The ultimate goal of these synthetic projects is to develop enantioselective routes to these complex molecules in sufficient quantities that are amenable for biomedical investigations.

Invited Lectures

Dr. Farukh Arjmand

Associate Professor, Department of Chemistry, Aligarh Muslim University, Aligarh-202002, India
Tel: 0571-2703893
E-mail: farukh_arjmand@yahoo.co.in

Academic Record

1986	Bachelors degree, University of Kashmir (J&K), India
1989	Masters in Chemistry, Aligarh Muslim University, (A.M.U.), Aligarh, India
1990	M.Phil, A. M. U., Aligarh, India
1993	Ph.D. in Chemistry, A. M. U., Aligarh, India, Title of M.Phil and Ph.D: "Synthesis, Characterization and Biocidal activity of Heterobimetallic Chelates"
1994-1998	Lecturer, Department of Chemistry, A. M. U., Aligarh
1998-2003	Senior Lecturer
2003-till date	Associate Professor

Awards

Shiksha Rattan Puraskar 2010, IFSI ,New Delhi

Membership in Professional bodies

Chemical Research Society of India (CRSI) (Life member)
Indian Council of Chemists (ICC) (Life member)
Indian Society of Chemists and Biologists (ISCB) (Life member)

Research Areas

- Synthesis and characterization of Heterobimetallic complexes
- Design and synthesis of new Chiral / achiral metal-based inorganic medicinal agents, in particular antitumor chemotherapeutic agents.
- In vitro metal complex- DNA/ nucleotides/ Protein (HSA, BSA) Interactions.

Projects Completed

1. Third World Academy of Sciences (TWAS) Italy (1995-96)
2. Council of Scientific & Industrial Research, (CSIR) New Delhi, India (2001-04)
3. University Grants Commission, New Delhi, India (2003- June 06)
4. Council of Scientific & Industrial Research, (CSIR) New Delhi, India (2005-08)

Reviewer

International Journal of Biological Macromolecules, Journal of Coordination Chemistry, European journal of Medicinal Chemistry, Spectroscopy Letters, Archiv di pharmie, Chirality, Journal of Applied Organometallic Chemistry, Journal of Photochemistry and Photobiology B: Biology, Nucleosides, Nucleotides, and Nucleic Acids, Molecular Biosystems Peer Reviewer for DBT, New Delhi sponsored research proposals.

Invited Lectures

New perspectives in cancer chemotherapeutic drug design: Effect of metal ions, ligand topology and chiral discrimination

Farukh Arjmand
Department of Chemistry, Aligarh Muslim University, Aligarh-202002, India.
E-mail: farukh_arjmand@yahoo.co.in

ABSTRACT

Medicinal inorganic chemistry is an interdisciplinary research area of growing interest in particular, for the diagnosis and therapy of cancer . Chemotherapy has greatly increased survival rates of cancer patients worldwide, therefore, besides other methods of treatment (surgery, radiotherapy etc.), chemotherapy still remains the most widely used treatment regime for controlling malignancies . Mechanistic details of cellular uptake and mode of action of cancer chemotherapeutics are not elusive, hence newer modalities in drug design are sought to offer. Metal-based drugs are more specific - target oriented, due to their tunable electronic and redox properties, DNA binding ability, relatively high affinity for nucleobases(in case of transition metal ions).Ligand topology plays a key role in the design of cancer chemotherapeutic agents. Appropriate multidentate ligand with a biologically active pharmacophore can offer chelation and also deliberate the functionality to induce tumor inhibition .While chelation removes the undesirable metal ions and can deactivate either the carcinogenic metal or the enzyme which is necessary for rapid growth of both the healthy and malignant cells, the biologically active functional groups can improve pharmocokinetic response and can facilitate cell- uptake , thereby enhance therapeutic potential of drug entities.. Among the other factors governing the binding modes, the most significant and fascinating criteria for drug design is the molecular shape-chiral preference or enantioselectivity. The best way to interact with nature is by using chiral molecules Literature reports reveal that the complexes that fit best against the DNA helical structure display the highest DNA binding affinity . New molecules which are marketed as efficacious drugs are single isomer drugs as they exhibit fewer side effects, and are more potent than their racemates.

Invited Lectures

Prof. Diwan S. Rawat

Professor, Department of Chemistry, University of Delhi, Delhi-110007, India
E-mail: dsrawat@chemistry.du.ac.in

Diwan S Rawat did master 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 50 research papers, authored a book, three book chapters, and four patents to his credit. His research interests lie in the areas of development of small organic molecules as anticancer, antimalarial and antimicrobial agents.

Prof. Rawat is a recipient of CRSI young scientist award (2007), ISCB young scientist award (2010) and Prof. D. P. Chakraborty 60th 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* and also serves on the Editorial Advisory Board of *Anti-Cancer Agents in Medicinal Chemistry,* and *Marine Drugs*.

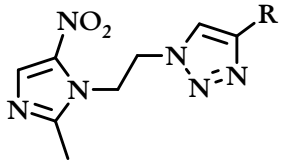
Invited Lectures

Synthesis and antimicrobial activity evaluation of cyclohexane-1,2- and 1,3-diamine derivatives and metronidazole–triazole conjugates

Diwan S. Rawat*
Department of Chemistry, University of Delhi, Delhi 110007, India
E-mail: dsrawat@chemistry.du.ac.in

ABSTRACT

Most of the antibacterial drugs in the clinical use have been discovered by the middle of last century and no new class of antibacterial was introduced in the market after 1962 until the discovery of linezolid in 2000.[1-3] Interestingly bacteria have developed resistance against most of these drugs soon after or even before their introduction in the market and multi-drug resistant has reached to the alarming stage[4,5] To overcome the antibiotic resistant problem, there is an urgent need for the development of new antibacterial class that are not affected by resistance mechanisms already present in the bacterial population.[6,7] As a part of our ongoing efforts towards the synthesis of novel antimicrobial agents,[8,9] we became interested to modify the metronidazole, a drug of choice for the treatment of anti-infectious diseases against protozoa such as *Trichomonas vaginalis*, *Entamoeba histolytica*, *Giardia intestinalis*, and infections caused by Gram-negative and Gram-positive anaerobes,[10,11] and bromhexine molecule, a mucolitic agent used in the treatment of respiratory disorders associated with viscid or excessive mucus. Careful structural modification of these two classes of compounds leads to discovery of potent antimicrobial agents.[12-14] The detailed synthetic methodology and antimicrobial activity of these compounds will be presented.



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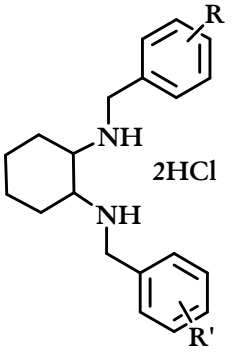

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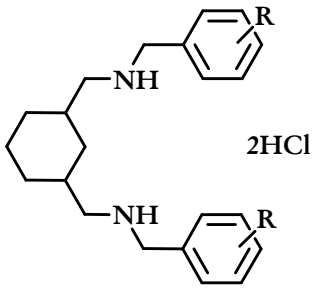


IC_{50} = 0.0006-0.4618μg/mL

Invited Lectures

Dr. Kishor S. Jain

Dean, Faculty of Pharmacy, Sinhgadh College of Pharmacy, Pune, India

Dr. Kishor S. Jain is B.Pharm. from Bombay University, Bombay, and M.Pharm. and Ph.D. (Medicinal Chemistry) from Gujarat University, Ahmedabad, India. Presently, he holds the posts of Principal and Professor of Medicinal Chemistry at Sinhgad College of Pharmacy, Pune, India. He has a total 20 years teaching & 10 years of Industrial experience. Earlier, he was Vice-President (R&D) of Dishman Pharmaceuticals & Chemicals Ltd, Ahmedabad. Gujarat, India as well as Director for a self owned Chemical CRO.

His areas of research include N.D.D.R. involving rational drug design, synthesis, and evaluation of novel antihyperlipidemeic, antihypertensive, anticancer, antimalarial antimicrobial and antiulcer agents. He also has considerable work in the field of Green Chemistry involving Microwave, based Chemical Synthesis and Phase Transfer Catalysis. He is also involved in Chemical Process development of API and specialty fine chemicals, Library synthesis, Custom synthesis, *etc*.

He has more than 60 research publications to his credit. He has filed two patents. He has written several quality reviews in international and national peer reviewed scientific journals. Notable are listed below. He has 2 Textbooks to credit and several major Research Projects (from Govt & University) received & successfully implemented so far.

He has presented more than 150 scientific papers at various conferences and symposia. Dr Jain has a Unique Blend of Applied as well as Basic Research Experience at Industrial & Academic levels, coupled with excellent communication and presentation skills & technical expertise. He is a good teacher and an excellent orator, who can present a topic in very comprehensive and lucid manner and keep the audience enthralled for hours even for a technical topic! He has delivered lectures at various places in the country as well as abroad. He was awarded the "Best Teacher of the Year 2004 " award by the 54th Indian Pharmaceutical Trust, Pune.

He was also Involved in Internal Quality Audits for GMP, ISO and also preparation for US-FDA inspections and had exposure in preparing Drug Master Files, Dossiers for Certificates of Suitability and Writing Technical Expert Reports for DMF's

He is a recognized PG and Ph.D. guide for five Universities. He has received several awards for best research papers and presentations at various conferences. *Recently, three of his research papers in IJPER, IJPS & Indian Drugs have received best paper awards at national levels in Oct, Dec 2009 & Jan 2010, respectively.* He is also a reviewer for some reputed international and national scientific journals.

He is currently the Member of American Chemical Society (ACS), Life-Member of Indian Pharmaceutical Association (IPA), Indian Society of Technical Education (ISTE), Association of Pharmacy Teachers of India (APTI), and Member of Board of Studies and Faculty of Pharmacy, Pune, University. He was also the Secretary of the IPA-Pune Branch and Member of National Executive Council of APTI. He was the Jt Secretary, LOC and key member of core committee for the organization of the 54th IPC, Pune in 2002. He has been Quoted in Marcus Who's Who-2008 for his quality research.

Currently, Dr Jain is the Dean, Faculty of Pharmacy, as well as, member, Academic Council, Univ. of Pune.

Invited Lectures

Novel conversion of multistep reactions into rapid one pot MCR under MWI for synthese of potentially bioactive heterocycles

K.S.Jain
Dean, Faculty of Pharmacy, Sinhgadh College of Pharmacy, Pune, India

ABSTRACT

New Drug Discovery Research holds key position in medicinal chemistry and health sciences. To discover a new drug approximately 1500 million US $ and 15-20 years required. About 10^4-10^5 new compounds need to be synthesized. In today's world speed is the essence for success and both synthesis and biological testing are automated and high throughput. Microwave irradiation (MWI) has really turned out to be a boon to organic synthesis in recent 10 years. Reactions can be completed in few minutes under MWI and the technique also falls under Green Chemistry. The present work is a successful attempt for the ultra-rapid one pot MWI based synthesis of a variety of potentially bioactive heterocycles (I, II, III, IV,V,VI). The compounds from these series have exhibited great potential for antihyperlipidemic (I-II), antiulcer (III), antitumor-anticancer (IV), and antifungal & antimicrobial (V-VI) activities. This methodology has been successfully made adaptable to automated parallel synthetic protocol. The reaction rates for entire multistep synthesis have been reduced from 6 – 48 hrs to just 10 -50 minutes! This has been achieved by judicious selection of reactants, reagents, solvents, reaction conditions and MWI technique.

Invited Lectures

Dr. Michael Pollastri

Associate Professor, Medicinal Chemistry and chemical technology, Department of Chemistry and chemical biology, Northeastern University, U.S.A.

Short biographical sketch

Michael Pollastri received his PhD from Brown University, his MS from Duke, and his bachelor's degree in chemistry from the College of the Holy Cross. After nine years working in medicinal chemistry and chemical technology at Pfizer's Groton and Cambridge sites, he transitioned in 2007 to an academic role at Boston University, where he established and operated the Center for Molecular Discovery, a combined medicinal chemistry and high-throughput screening center. In 2009 he joined the faculty at Northeastern University in the Department of Chemistry and Chemical Biology as Associate Professor, where his research is primarily focused on drug discovery for neglected tropical diseases.

Invited Lectures

Target repurposing for neglected tropical disease drug discovery

Michael Pollastri

ABSTRACT

Parasitic diseases such as African sleeping sickness, leishmaniasis, and Chagas disease affect a significant patient population in developing countries. Since recovery of research costs for discovering drugs for these diseases would be challenging, drug discovery efforts for these diseases fall primarily to the not-for-profit sector. However, the mindset and technologies employed in industry that enable efficient optimization of small molecule therapeutics are not widely practiced in the academic environment. Our efforts in establishing an industrial outpost of hit-to-lead medicinal chemistry in academia will be described, using examples of our drug repurposing approach to highlight the pragmatic strategies and technologies we apply.

Invited Lectures

Dr. Vibha Tandon

Associate Professor, Department of Chemistry, University of Delhi
Tel: 91-11-27667725, ext: 1347, 1375, 91-11-2766646, ext: 174, 144
E-mail: vtandon@acbr.du.ac.in; vibhadelhi@hotmail.com

List of Positions Held

- January 2009 - Reader in Department of Chemistry
- January 1998-2009: Research Scientist (Lecturer), University of Delhi, Delhi –110 007.
- January- December 1997: Production In charge of a 100% EOU producing Surgical Gloves i.e. M/S KCK Latex Limited, Delhi.
- April 1996- December 1996: Senior Chemist of an 100% EOU producing Surgical Gloves i.e. M/S KCK Latex Limited, Kanpur & Delhi.

Sponsored R& D Projects

Projects Completed

1. Project Title: Antisense Oligonucleotides as Chemotherapeutic Agents: Physico –Chemical and Biological Studies (PI)
   Funding Agency: DST. Amount: 8 Lakhs. Duration: 2001-03.
2. Project Title: Synthesis of Oxandrolone,
   Funding Agency: Hikma Pharmaceuticals, Jordan. Amount: $ 15000. Duration: 2002 –2003.
3. Project Title: Inhibition of HIV-1 replication: Design, Synthesis and Characterization of Small Molecule Libraries.(Co–PI)
   Funding Agency: UGC; Amount: 9.5 Lakhs. Duration: 2004-2007.
4. Project Title: Structure Activity Relationship Studies of Marine Natural Products – Apratoxins, (PI)
   Funding Agency: UGC; Amount: 4.6 Lakhs, Duration: 2004-2007.
5. Project Title: "Drug target validation and antiinfective Development for HIV/AIDS and associated infections"
   Funding Agency: Swedish International Development Cooperation Agency (SIDA) under the Asian-Swedish Research Partnership Programme; Amount: Total 324 000 SEK. Duration: 2005 -2007.
6. Project Title: Nutritional & Hypoglycemic effect of Fruit Pulp & Leaves of *Annona squamosa*.
   Funding Agency: ICMR; Amount: 4.76 Lakhs, Duration: 2002 –2005.
7. Project Title: Identification and Characterization of Antidiabetic compounds from *Annona squamosa* and *Ocimum sanctum*.
   Funding Agency: ICMR; Amount: 11.50 Lakhs, Duration: 2005-2008.
8. Project Title: Synthesis and Characterization of DNA Minor Groove Binding Ligands for Biological Applications.
   Funding Agency: INMAS, DRDO; Amount: 11.20 Lakhs, Duration: 2005-2008.
9. Project Title: Investigation of the Characteristics of the Biologically Active Systems Using the Probes showing Proton Transfer & Electron Transfer Behaviours: Synthesis and Photophysics
   Funding Agency: DST; Amount: 25 Lakhs. Duration: 2005-2008.

Research Areas

Medicinal Chemistry, Oligonucleotide Therapeutics, Radiation, Biology, Natural Products.

Invited Lectures

A systematic study of benzimidazoles in search of selective antimicrobials targeting topoisomerase I: Development of *E.coli*. inhibitors

Vibha Tandon
Department of Chemistry, University of Delhi
E-mail: vtandon@acbr.du.ac.in

ABSTRACT

New antimicrobials are needed to combat drug resistance. One attractive strategy is to develop ligands to selectively target microbial DNA over host DNA. DNA minor groove binders already provide useful antimicrobial and antitumour agents, however, their cytotoxicity in mammalian systems limits applications. Recently, we reported bisubstituted analogues of benzimidazoles with impressive DNA affinity yet surprisingly low mammalian cytotoxicity. Here we tested the antimicrobial effects of bisubstituted analogues of Hoechst 33342 and observed overall impressive antimicrobial effects against gram negative, gram-positive bacteria, and fungi. Furthermore, the most potent ligand, DMA (benzimidazole) cleared bacterial infections from mammalian cell cultures without apparent inhibition of the mammalian cells. The bisubstituted ligands preferentially inhibit bacterial topoisomerase I relative to mammalian topoisomerase *in vitro*, suggesting that selective topoisomerase poisoning underlies the selective antibacterial effects. This is in principle, of considerable interest as specific inhibitors of bacterial topoisomerase I are not known till date. Lower MIC values and longest duration of postantibiotic effect amongst the tested antibiotics favours the development of benzimidazoles as potent antibacterial agents. One of the putative target of the synthesized molecules is topoisomerase I. Fluorescence titrations also suggested that benzimidazoles bind reversibly to topoisomerase I and do not stabilize cleavable complexes. Our results also suggested that benzimidazoles bind directly to enzyme with high affinity. Benzimidazoles do not inhibit DNA gyrase but inhibits mammalian topoisomerase II but at very high concentrations. We have also observed that benzimidazoles are inhibitors of Camptothecin resistant human topoisomerase I, increasing the clinical relevance of benzimidazoles.

REFERENCES

[1] Manish Singh, Vibha Tandon. European Journal of Medicinal Chemistry. European J. of Medicinal Chemistry (EJMECH-D-10-00384R2). Accepted.
[2] Sandhya Bansal, Vibha Tandon. International J. of Antimicrob. agents (IJAA-D-10-00767), Accepted.
[3] Sandhya Bansal, Urmila Tawar, Manish Singh, Abbas Nikravesh, Liam Good, Vibha Tandon. International J. of Antimicrob. Agents 2010, 35: 186-190.
[4] Akash K. Jain, Sharad K. Gupta, Vibha Tandon. Oligonucleotides, December 2009, 19(4): 329-340.
[5] Akash K. Jain , Sharad K. Gupta, Urmila Tawar, Sneh K. Dogra, Vibha Tandon. Oligonucleotides, March 2009, 19(1), 53-62.
[6] U. Tawar, S. Bansal, S. Shrimal, M.Singh, Vibha Tandon. Molecular & Cellular Biochemistry 2007, 305(1-2), 221-23.
[7] Urmila Tawar, Akash K. Jain, B. S. Dwarakanath, Ramesh Chandra, Yogendra Singh, N. K. Chaudhury, Divya Khaitan and Vibha Tandon. Journal of Medicinal Chemistry 2003, 46, 18, 3785-3792.
[8] Urmila Tawar, Akash K. Jain, Ramesh Chandra, Yogendra Singh, B.S Dwarakanath, N.K. Chaudhury, Liam Good, Vibha Tandon . Biochemistry, 2003, 42, 13339-46.

Invited Lectures

Dr. Brajesh Kumar

Assistant Professor, Department of Chemistry, Tata College (Post Graduate College), Kolhan University/ Ranchi University, Chaibasa, West Singhbhum, Jharkhand 833-202, INDIA
Tel: 82-10-6429-5944 (M), 82-02-2049-6233 (O), 82-02-2450-4255 (R)
Email: krmbraj@gmail.com; krmbraj1@rediffmail.com; krmbraj@konkuk.ac.kr

Work Experience

- Assistant Professor March 2010-
  School of Life & Environmental Science, Konkuk University, Seoul, South Korea
- Assistant Professor March 2008 –
  Tata College (P.G. College), Kolhan University/Ranchi University, Chaibasa, Jharkhand, India
- Guest Lecturer August 2007 – March 2008
  Acharya Narendra Dev College (ANDC), Govindpuri, University of Delhi, Delhi, India
- Guest Lecturer October 2007 – March 2008
  Rajdhani College, Raja Garden, University of Delhi, Delhi, India

Research Interests

- Development of Sustainable and Ecofriendly methods for Natural Product Extraction, Purification and Analysis.
- Microwave and Ultrasound Assisted organic synthesis, One Pot Synthesis, Chromatography, HPLC, Spectra Analysis (NMR, IR, LC-MS, UV-Visible)
- Multistep organic synthesis (solid & solution phase) in small scale & large scale, Linear and Cyclic Peptide synthesis, N-Methyl amino acid, Peptide Nucleic Acid (PNA), & Locked Nucleic Acid (LNA) synthesis
- Medicinal Chemistry

Honors and Awards

- Life Member - Indian Society of Chemists and Biologists (ISCB), India
- Reviewer – Advanced Materials Letters (A peer reviewed international journal of material science)
- CSIR-UGC National Eligibility Test, NET (18/12/2005 & 18/6/2006)
- Graduate Aptitude Test Examination, GATE (2004 & 2006)

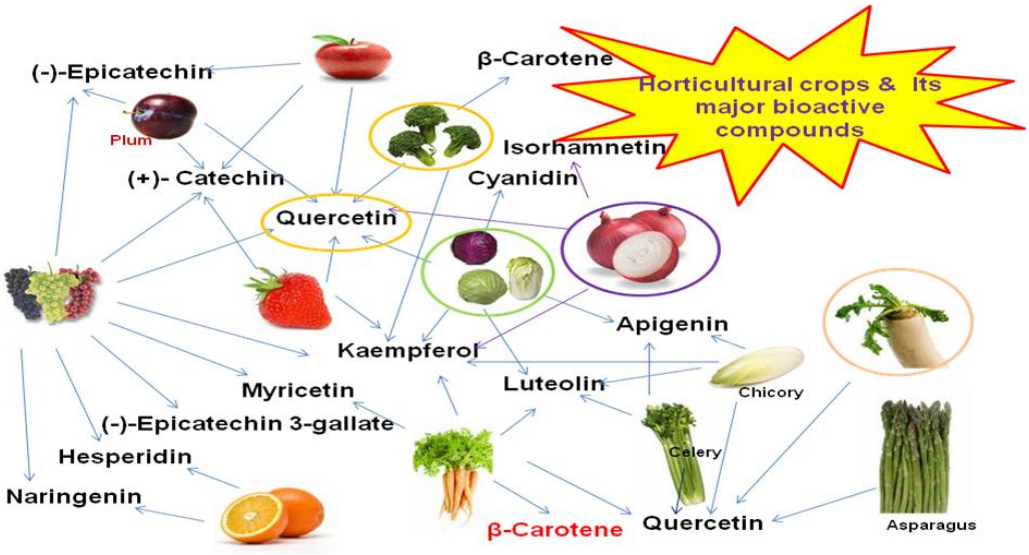
Invited Lectures

Environmentally sustainable technique for production of bioactive compounds from agriculture wastes

Brajesh Kumar[1,2] and Se Won Park*[,1]
[1]Department of Molecular Biotechnology, School of Life and Environmental Science, Konkuk University, Seoul, Republic of Korea
[2]Tata College, Department of Chemistry, Kolhan University, Chaibasa, Jharkhand, India
E-mail: krmbraj@gmail.com

ABSTRACT

The agricultural, forestry, and food industries produce tons of waste materials and by-products every year, such as onion skin, apple peel, carrot waste and birch bark. The produced waste and by-products are today used in animal feed, or for composting, incineration or anaerobic digestion. However, these waste materials and by-products contain high-value compounds such as antioxidants that can be extracted before the waste reaches its final destination. Waste and by products from fruits and vegetables are rich in antioxidants such as polyphenols, which have uses as additives in pharmaceuticals, food products and cosmetics. Now a day, extraction techniques have been widely investigated to obtain such valuable natural compounds from agricultural wastes for commercialization. In addition, these extracted compounds are further modified to other bioactive compounds. The development of faster, simpler, inexpensive and more environmentally-friendly extraction and separation techniques is an important issue in food chemistry. Quantitatively microwave-assisted extraction (MAE), ultrasound-assisted extraction (MAE) and ionic liquid-based extraction is an improved extraction method with high efficiency in extraction time and environmental-friendliness.



Invited Lectures

Dr. Akhilesh Kumar Verma

Associate Professor, Department of Chemistry, University of Delhi, Delhi-110007, India.
Tel.: 91-11-27666646 (Ext.175), 09717831262
E-mail: averma@acbr.du.ac.in
Web page: www.akvresearch.com

Academic

Associate Professor: March 2010-till date Department of Chemistry, University of Delhi (Post-graduate level)
Reader: Jan 2009-March 2010 Department of Chemistry, University of Delhi (Post-graduate level)
Lecturer: Jan 1998-jan 2009 Dr. B.R. Ambedkar Center for Biomedical Research, University of Delhi, Delhi (Post-graduate level)

Honors / awards

- Invited by National Organic Symposium Trust (NOST) for a talk in NOST XIV Organic Chemistry Conference (Will be held in Goa between December 5-8, 2010)
- Invited by Editor of Wiley-Blackwell for the Coauthor ship for Editing the 3rd Revision of Comprehensive Organic Transformation (COT-III)
- Awarded BOYSCAST Fellowship for one year (2007-2008) in the laboratory of Prof. R. C. Larock at Iowa State University of Science and Technology, Ames, Iowa, USA for the advance research.
- Awarded Post Doctoral Fellowship by the Dept. of Chemistry, University of Florida, Gainesville, USA, for one year (Jan 2001-Dec. 2001) in the Laboratory of Prof. Alan R. Katritzky.
- Awarded Post Doctoral Research Associate fellowship by the Dept. of Chemistry, University of Florida, Gainesville, USA, for one year (Jan 2001-Dec. 2001) in the Laboratory of Prof. Alan R. Katritzky.
- International Conference on Recent Advances in Biomedical and Therapeutic Sciences (13th – 15th Jan, 2004) organized by Bundelkhand University, Jhansi in Collaboration with University of Nether land in Jhansi, INDIA. (*Best poster award*)

Areas of Interest

Synthetic Organic Chemistry / Bioorganic Chemistry

Sponsored Research Projects

1. Title of the Project: "Design and Synthesis of New class of DNA intercalating agents" Funding agency: Delhi University (PURSE Grant) Amount: 28.7 Lakhs Duration: Three year (2009-2010)
2. Title of the Project: "Design Synthesis and biological evaluation of novel integrase" Funding agency: DST Amount: ~36.0 Lakhs Duration: Two year (2009-2012) Role: Co-Investigator
3. Title of the Project: "Design Synthesis and antibacterial studies of novel 1,2,3,4tetrahydropyrazino[1,2-a]indoles on resistant bacterial strains" Funding agency: DST Amount: 20.38 Lakhs Duration: Two year (2009-2010)
4. Title of the Project: "Design of Tandem and selective synthesis of α-fused polycyclic quinoxalines" Funding agency: UGC Amount: 8.84 Lakhs Duration: Three year (2009-2010)
5. Title of the Project: "An Efficient Assembly of Heterobenzazepines and tetrahydropyrazino indoles ring system by intramolecular cyclization by benzotriazole methodology" Funding agency: DST Amount: 12 Lakhs Duration: Three year (2003-2006)
6. Title of the Project: "Green & Environment Friendly approach for the construction of potential heterocycles" Funding agency: DRDO Amount: 14.4 Lakhs Duration: Two year (2006-2008)

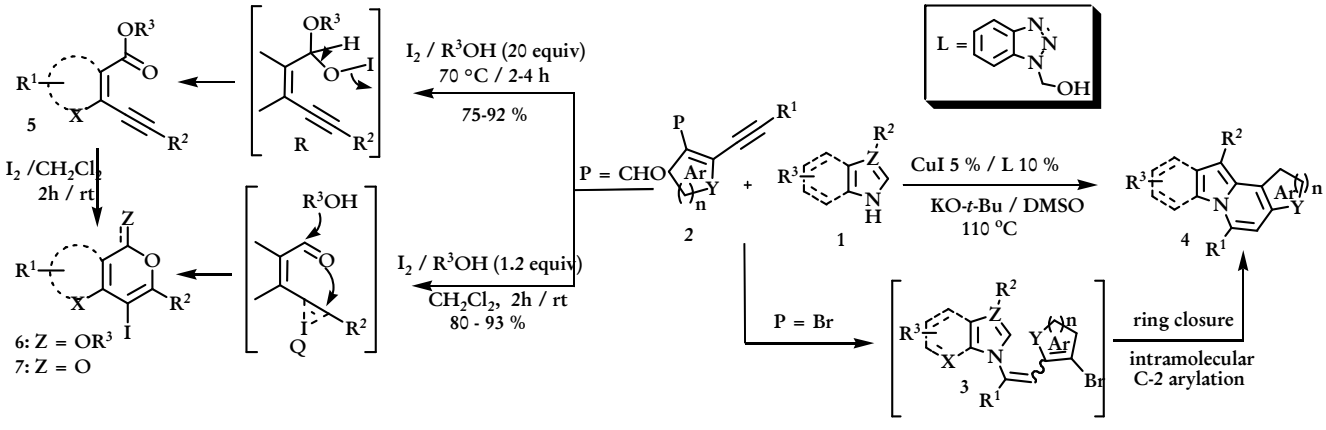
Invited Lectures

Tandem synthesis of indolo-, pyrrolo[2,1-*a*]isoquinolines, naphthyridines, pyranoquinolines, pyranoquinolinones and isocumarins by the electrophilic cyclization of alkynes

Akhilesh Kumar Verma
Synthetic Organic Chemistry Research Laboratory, Department of Chemistry, University of Delhi, Delhi-110007, India
E-mail: averma@acbr.du.ac.in

ABSTRACT

Nitrogen heterocycles indolo[2,1-*a*]isoquinoline has a unique nitrogen containing tetracyclic structure, characteristics of dibenzopyrrocoline alkolids, cryptaustoline P and cryptowpline Q isolated from the bark of Cryptocarya bowiei, which are reported to possess antileukemic, tublin polymerization inhibitory and antitumour activities[1a-d]. Polyheterocycles 4 were synthesized regioselectively in one pot by the copper-catalyzed tandem addition of *N*-heterocycles 1 onto *ortho*-haloarylalkynes 2, followed by intramolecular arylation without isolating intermediate 3. This chemistry appears to involve the preferential nucleophilic addition of *N*-heterocycles onto the *ortho*-haloarylalkynes over *N*-arylation of the aryl halide[2a-d]. Oxygen heterocycles pyranoquinoline, pyranoquinolinone and isocumarin moiety is known to be present in many alkaloids, and possesses a wide range of pharmacological activities and biological activities like anticoagulant, coronary constricting, optical brightening, antifungal, antihistamine and anti allergic activities[3a-d]. *Ortho*-alkynyl aldehydes, on reaction with I_2 in CH_2Cl_2 with appropriate nucleophiles provides pyrano[4,3-*b*]quinolines 6, via formation of cyclic iodonium intermediate Q, however using alcohols as a solvent as well as nucleophile, *ortho*-alkynyl esters 5, were obtained selectively in good to excellent yields via formation of hypoiodide intermediate R. Subsequently, *ortho*-alkynyl esters 5 were converted in to pyranoquinolinones and isocoumarin 7 by the electrophilic iodocyclization[4a-c].



Invited Lectures

Dr. Arun Kumar Shaw

Division of Process and Medicinal Chemistry, Central drug Research Institute, CSIR, Chatter Manzil, Lucknow-226 001
E-mail: akshaw55@yahoo.com

M.Sc. in Chemistry (Organic), University of Calcutta, 1977.

Ph. D., University of Calcutta, 1985 with Professor Subhendu N. Ganguly at Bose Institute, Calcutta in. After his doctoral work he also worked with Professor S. K. Talapatra in the Department Of Pure Chemistry, University of Calcutta from October 1985 to January 1987.

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

Visit to abroad

Faculty of Chemistry, Dept of Organic Chemistry University of Rostock, and Rostock three months from April' 2000 to June' 2000 *Under CSIR-DAAD Exchange of Scientists programme*

Research Area

Medicinal Chemistry, Natural Products Chemistry and Chiron Approach Synthesis of bioactive natural products or natural product like molecules, development of new methodology/synthetic reagents and investigation of new reaction pathways in Organic Synthesis

Number of Ph.D supervised

Five and currently supervising seven students for their Ph.D degrees.

Number of Publications

More than forty research papers to various journals of national and International repute.

Invited Lectures

Chiron approach synthesis of natural products and natural product like molecules from carbohydrate-based building blocks

Arun K. Shaw
Division of Process and Medicinal Chemistry, Central drug Research Institute, CSIR, Chatter Manzil, Lucknow-226 001
E-mail: akshaw55@yahoo.com

ABSTRACT

Despite being a rich source of energy and also having multiple well defined chiral centres, carbohydrates are considered to be very versatile building blocks for stereoselective synthesis of various natural product and natural product like molecules. This approach of synthesis of target molecules is popular as "Chiron approach synthesis". However, the right choice of carbohydrate as a synthon depends on the structure of the target chiral molecule. For the last few years our group has been working towards Chiron approach synthesis of biologically active various Natural products and Natural product like molecules using commercially available carbohydrates as "chiral pools". We have also focused on development of new methodology to access some "carbohydrate-based chiral building blocks" (CBBs) and latter used them for the synthesis of targeted natural products and biologically relevant molecules. A summary of work done in our laboratory on stereoselective synthesis of various molecules and natural products of biological importance using commercially available carbohydrates as chiral synthons will be presented.

Invited Lectures

Dr. P.M.S.Chauhan

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

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 Jan.-June 2003, (16 months):	Visiting Scientist, School of Chemical Sciences, University East Anglia, Norwich, UK

Field of Specialization

Synthetic Organic chemistry/Medicinal chemistry, (26 Years), Combinatorial chemistry (11 Years)

RESEARCH EXPERIENCE AND POSITIONS HELDS

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

HIGHLIGHTS OF RESEARCH ACTIVITIES

Paper published in peer reviewed Journals	90
Patents (Indian) Filed	6
Ph. D. Thesis supervised	11

Honors and Awards

1. Recipient of the CDRI incentive award for the year 2000.
2. Recipient of the CDRI incentive award year for the 2001.
3. Fellow of Royal Society Chemistry(FRSC) ,2003
4. AWARD for outstanding contributions in Medicinal chemistry and international scientific collaboration (Scientific Partnership Foundation,Moscow,Russia,2005).
5. Rashtriya Gaurav Award, 2010, Indian International Friendship Society, New Delhi
6. Member Editorial board , *Future Medicinal Chemistry, Future science group*
7. *Most Cited paper,(2005-2008) award by Elsevier Bioorganic & Medicinal Chemistry Letters).*
8. Recipient of the CDRI incentive award year for the 2010.
9. Deliver Keynote Lecture, 42nd IUPAC /RSC Conference on Aug.,2nd -7th 2009 , Glasgow, UK

Organizing capabilities

8 National conferences, 6 international conferences were organized as General Secretary of Indian society of Chemists and Biologists, CDRI, LUCKNOW,(Website; www.iscbindia.org) .This year Prof. Robert H. Grubbs, *Nobel laureate has delivered his lecture in ISCB-2010.*

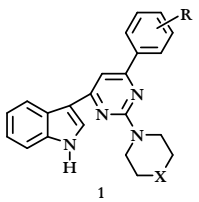
Invited Lectures

Design and synthesis of nitrogen heterocycles as novel therapeutic agents

P.M.S.Chauhan
Medicinal and Process Chemistry Division, Central Drug Research Institute Lucknow, India 226001
E-mail: premsc58@hotmail.com; prem_chauhan_2000@yahoo.com

ABSTRACT

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 [1-10]. 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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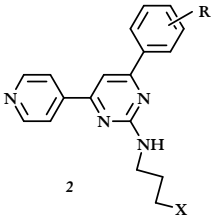

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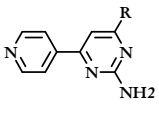

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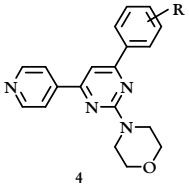

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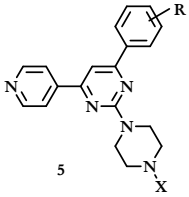

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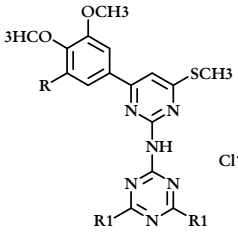

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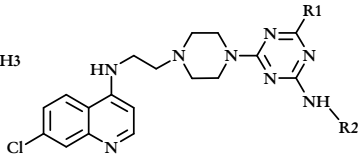

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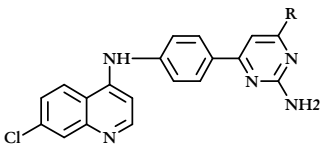

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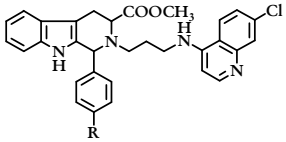

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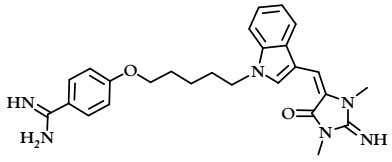

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Invited Lectures

Prof. Dalip Kumar

Department of Chemistry, Birla Institute of Technology & Science, Pilani-333 031, Rajasthan
Tel: +91-1596-245073-279
Fax: +91-1596-244183
E-mail:dalipk@bits-pilani.ac.in

Present Position

Associate Professor & Head of Department, BITS, Pilani

Research Area

Synthetic Organic and Medicinal Chemistry

Education

- Ph.D. (Organic Chemistry), 1997, Kurukshetra University Kurukshetra, Haryana
- M. Phil. (Organic Chemistry), 1993 Kurukshetra University Kurukshetra, Haryana

Teaching and Research Experience

2004-10 Assistant Professor & Head of Department, BITS, Pilani
2002-04 Research Associate, Dept of Chemistry & Biochemistry, UMD, College Park, USA 2000-02 Lecturer, Dept of Chemistry, BITS, Pilani
1999-00 Post-doctoral Fellow, Medicinal Chemistry Division, UT, Austin, USA
1997-99 Postdoctoral Fellow, Sam Houston State University, Huntsville, TX, USA

Publications

Research Papers : 65
Patent : 02
Invited Lectures : 10

Invited Lectures

Indolyl azoles as novel and selective anticancer agents

Dalip Kumar
Department of Chemistry, Birla Institute of Technology & Science, Pilani
E-mail: dalipk@bits-pilani.ac.in

ABSTRACT

A large number of indolyl azoles isolated from different microorganisms are reported to display interesting biological activities [1-3]. There are many natural and synthetic indole-based heterocycles with diverse mechanism of action have been reported as lead anticancer molecules [2]. The Labradorin 1 and Labradorin 2 are isolated from *pseudomonas syringae pv. Coronafaciens*, are known to exhibit significant inhibitory activity against various human cancer cells [3]. Isolated from marine sponges, the natural bis(indole)alkaloids such as topsentin and nortopsentins were demonstrated significant *in vitro* cytotoxicity against P388 cells [1]. There are many indole-based compounds found to be effective as tubulin assembly inhibitors, particularly, recently reported 3-aryl-thioindoles have displayed significant cellular apoptosis [4]. Indolylthiazoles were evaluated for their cytotoxic activity against human breast tumor cell lines. A thiazolyl indolequinone, BE 10988, isolated from culture broths of Streptomyces strain, is known to increase DNA-topoisomerase complex formation and displayed significant anticancer activities [5]. Encouraging activities of indolyl azoles prompted us to investigate new analogues with further modification of five-membered heterocyclic ring and indolyl moiety to optimize the structure-activity relationship (SAR) leading to potent and selective anticancer agents [6]. We have designed and synthesized a series of indolyl azoles which are selectively cytotoxic against human cancer cells. Recent results from our laboratory will be presented in the conference.

REFERENCES

[1] P P Diana, A Carbone, P Barraja, M A Montalbano, G Dattolo, O Gia, L D Viab and G Cirrincione, Bioorg. Med. Chem. Lett. 17, 2007, 2342.
[2] S R Naik, J Harindran and A B Varde, J. Biotechnol. 88, 2001, 1.
[3] G R Pettit, J C Knight, D L Herald, H R Davenport, R K Pettit, B E Tucker and J M Schmidt, J. Nat. Prod.65, 2002, 1793.
[4] G D Martino, G L Regina, A Coluccia, M C Edler, M C Barbera, A Brancale, E Wilcox, E Hamel, M Artico and R Silvestri, J. Med. Chem. 47, 2004, 6120.
[5] C J Moody, E Swann, S Houlbrook, M A Stephens and I J Stratford, J. Med. Chem. 38, 1995, 1039.
[6] **(a)** D Kumar, N M Kumar, S. Sundaree, E O Johnson and K. Shah, Eur. J. Med. Chem. 45, 2010,1244. **(b)** D Kumar, N M Kumar, K Akamatsu, E Kusaka, H Harada and I Takeo, Bioorg. Med. Chem. Lett. 20, 2010, 3916. **(c)** D Kumar, N M Kumar, K-H Chang and K Shah, Eur. J. Med. Chem. 45, 2010, 4664. **(d)** D Kumar, N M Kumar, K-H Chang and K Shah, Chem. Biol. Drug. Des. 2010 (Accepted).

Invited Lectures

Dr. Wahajul Haq

Scientist F
Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow 226 001
E-mail: w_haq@cdri.res.in

Educational Qualifications

Degree	University	Year	Division	Subjects
B. Sc.	Bundelkhand University., Jhansi	1977	I	Zoology, Botany, Chemistry
M. Sc	Bundelkhand University., Jhansi	1980	I	Org. Chemistry
Ph.D.	Lucknow University, Lucknow	1989	-	Chemistry*

***Title :** Design and synthesis of peptides with immunomodulatory and antiviral activity.

Positions held

1982-1987	Research Fellow	Med. Chem. Division, Central Drug Research Institute, Lucknow
1988-2001	Scientist	Division of Biopolymers, Central Drug Research Institute, Lucknow
2001-till date	Scientist	Med. Chem. Division, Central Drug Research Institute, Lucknow

Visits Abroad

Visiting Scientist	Nov. 1991-Feb. 1992	Dept. of Chemistry, University of Arizona, USA
Visiting Scientist (DBT Overseas Fellow)	Jan. 1994-Feb.19 95	Dept. of Chemistry, University of Arizona, USA
Visiting scientist	August 22-26, 1995	Ferring Peptide Production AB, Malmo, Sweden
Visiting Investigator	June 2003-Nov. 2004	Beckman Research Institute, Duarte, CA, USA

Fields of specialization

Synthetic peptides & small organic molecules

Areas of interest

Design and synthesis of peptides of biomedical interest, Development of new synthetic methodologies for small organic molecule synthesis and combinatorial Chemistry

Number of Publications

More than 90 in peer reviewed journals

Patents

Indian Patent (17), US Patent (4) EU Patent (5)

Invited Lectures

Peptide-oligonucleotide conjugates as therapeutics

W. Haq
M. P. C. Division, Central Drug Research Institute, Lucknow 226 001
E-mail: w_haq@cdri.res.in

ABSTRACT

Peptides and Oligonucleotides constitute of potential therapeutic agents. The biological significance of peptides and proteins is very well studied and is better understood compared to that of oligonucleotides. In fact, many peptide and protein based therapeutics as well as vaccines are in use. Recent observations that synthetic oligonucleotides and their modified analogues can be used successfully to modulate the functions of specific genes, the research on oligonucleotide based therapeutics has been intensified. It is believed that therapeutics based on ligonucleotides will become a reality in the future. The peptide-oligonucleotide conjugates are reported to improve the basic problems associated with oligonucleotide as effective therapeutics viz. poor cellular uptake of naked oligonucleotides, low binding affinity to the target etc.. However, proper methodologies are yet to be developed for the preparation these up-coming novel therapeutic agents. The lack of straightforward method for chemical synthesis and further advancement in experimental protocols limits the realization of full potential uses of these novel bioconjugates. Vaccination strategies remain elusive that are effective against viral disease pathogens yet remain gentle enough for widespread human use. We developed a model system that relies on the recognition of specific T-cell epitopes from immunodominant antigens of HIV to explore single-stranded CpG-oligodeoxynucleotides (CpG-ODN) as an adjuvant. We improved upon current strategies of utilizing CpG in combination with peptide vaccines by covalently modifying epitope fusion peptides with CpG motifs. Immunogenicity of DNA–peptide conjugates was superior in sensitivity to non-covalently linked mixtures of the same functional molecules. Synthesis of fusion peptide conjugates with CpG-DNA fragments will be discussed.

Invited Lectures

Dr. Brijesh Kumar Srivastava

Scientist, Zydus Research Centre, Ahmedabad, India
Tel: +91-09427710112, +91-09327064704
E-mail: bksri2000@rediffmail.com; bksri2000@yahoo.com

Research Interest

Synthesis of biologically useful and interesting molecules of pharmaceutical importance, stereo selective synthesis of drug and drug intermediates, drug design and process development of new chemical entities (NCE).

Salient Features of Achievements in Industrial Research during 2001-Todate

- Since 2001, working in the Medicinal Chemistry Department of the Zydus Research Centre, Cadila Healthcare Limited, and involved in the synthesis of (i). novel oxazolidinones and quinolones as antibacterial agents (ii) cannabinoid modulators as antiobesity drug (CB1 antagonist) as well as antipain (CB2 agonist) compounds and (iii) Exploring newer targets for cardiometabolic and associated disorders.
- Main interests lies in the synthesis of biologically useful and interesting molecules of pharmaceutical importance, stereo selective synthesis of drug and drug intermediates, chiral resolution, drug design, and also the process development of New Chemical Entities.
- Filed several patent applications, published several papers in peer reviewed journals and contributed a chapter in a book *Comprehensive Heterocyclic Chemistry III*.
- Delivered several talks, participated in several international conferences and attended several workshops in the area of drug development.

Research Experience

2001-Todate	Syntheses of Novel oxazolidinone and Quinolone as Antibacterial Agents and Cannabinoid Receptor modulators as Anti obesity drug (CB1 antagonist) as well as anti pain (CB2 Agonist) compound in an Indian Pharmaceutical Research Organization
2000-2001	Novel process of fluconazole, acyclovir
1999-2000	One year teaching experience to post-graduate level

Awards and Fellowships

- *CDRI AWARD-2008 for Excellence in Drug Research*
  1994-1998 Research Fellow, Anti fertility Drug Development Scheme, Ministry of Health & Family Welfare, Govt. of India, New Delhi.
- 1993 Research Fellow (Indo-US, CONRAD Scheme), Dept. of Biotech, Govt. of India, New Delhi, India

Invited Lectures

Novel substituted 1H-benzo[d]imidazole-2-carboxamide derivatives as selective and oral CB2 agonists for the prevention of allodynia in rat neuropathic pain models

Brijesh Kumar Srivastava[†], Pravin Kadam[†], Shivaji Gugale[†], Sandeep Shedage[†], Umesh Mali[†], Praveen kumar Singh[†], Purvi Vyas[¥], Hitesh Bhayani[¥], Rakesh Patel[§], Rina Soni[†£], Jayendra Patel[†], Rahul Salunke[†], Sidhartha Kar[†], Priyanka Priyadarsiny[¥], Vishwanath Pawar[§], Mukul Jain[§] and Pankaj Patel[†]

[†]Dept of Medicinal Chemistry, [§]Dept of Pharmacology, [¥]Dept of Cell Biology.
Zydus Research Centre, Sarkhej-Bavla N. H. 8A, Moraiya, Ahmedabad- 382210, India.
[£]Present address: Dept of Chemistry, University of Warwick, UK.
E-mail: brijeshsrivastava@zyduscadila.com

ABSTRACT

There is growing interest in using CB2 receptor agonists for the treatment of neuropathic pain. Neuropathic pain can be a debilitating condition characterized by severe and persistent pain. In this presentation, we describe the pharmacological characterization of 1H-benzo[d]imidazole-2-carboxamide derivatives (fig.1), their functional activity and selectivity against human CB2 receptors using cAMP assay. The lead compound attenuated tactile allodynia produced by spinal nerve ligation (SNL) in a dose-related manner. These results show promise for this class of compounds as potent CB2 agonists in the treatment of neuropathic pain.

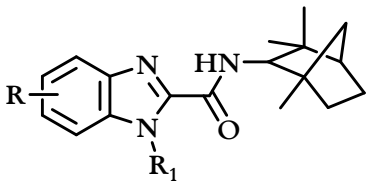


Figure 1: Novel Benzo[d]imidazole-2-carboxamide derivatives

Invited Lectures

Prof. Ashok K Prasad

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

Professor Ashok K Prasad graduated with a M.Sc. degree in Organic Chemistry in 1986, from Bihar University, Muzaffarpur. He obtained his PhD from University of Delhi in 1990 on synthesis of phenolic natural products and subsequently held postdoctoral positions at the Department of Physics & Chemistry, University of Southern Denmark, Odense, Denmark, University of Copenhagen, Denmark, etc and visiting researcher at Max-Planck-Institute for Molecular Physiology, Dortmund, Germany; UMASS, Lowell, USA, etc prior to joining Department of Chemistry, University of Delhi in 2001.

His major research interests include synthesis of modified nucleosides and oligonucleotides involving them and efficient methodology development using lipases as selective biocatalysts.

He is the 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)

Recently he has been the Guest editor of special issues of *Biochemie*, a journal published by Elsevier and *Indian Journal of Chemistry*, being brought by CSIR

He has been in the different scientific committees of DBT and DST

PUBLICATIONS

Professor Prasad published 130 Research Papers in the International Journal of Repute

PATENTS

He has three International Patents and three Indian Patents in his credit

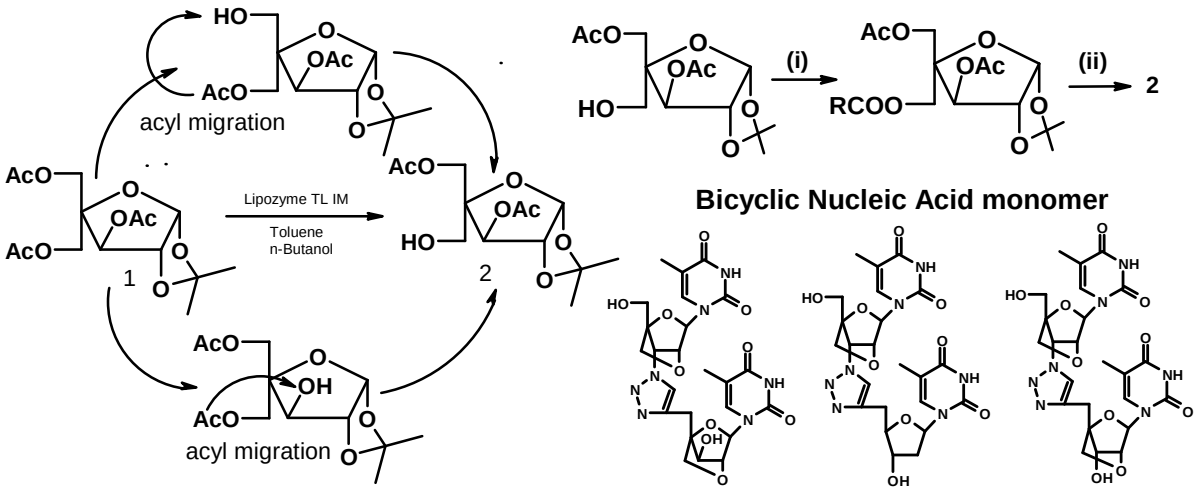
Invited Lectures

Sustainable route to modified nucleosides and non-ionic nucleoside dimers of importance in healthcare

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

ABSTRACT

One of the important components of Nucleic Acids is deoxyribose and ribose sugars. 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. The intrinsic problem in such synthesis is the selective manipulation of different hydroxyl and amino functions present in the compound under mild reaction condition. We have developed an efficient biocatalytic methodology for the selective manipulation of different hydroxyl groups in the sugar during the synthesis of nucleosides of biological importance. Detailed results will be presented in the meeting.



Invited Lectures

Prof. Brindaban C. Ranu

Senior Professor, Department of Organic Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Kolkata - 700032, India
E-mail: ocbcr@iacs.res.in
URL: http://bcranu.freehostia.com

Brindaban C. Ranu recieved his M.Sc. from Calcutta University in 1970 and obtained his Ph.D. from Jadavpur University in 1982 working with Professor U.R. Ghatak at Indian Association for the Cultivation of Science. He did his post-doctoral work in Virginia Tech, USA with Prof. T. Hudlicky during 1982-85 and started independent research at the department of organic chemistry, IACS from 1985. His current research interests lie in the area of green synthesis including development of green catalysts and green procedures for organic reactions. He has published more than 200 papers (205+) and supervised 23 Ph.D. students.

He is a fellow of the Indian Academy of Sciences and Indian National Science Academy. He is a recipient of J.C. Bose National Fellowship, DST, Govt. of India (2009-2014). He received N.S. Narasimhan Award in 1993 and Chemical Research Society of India Bronze medal in 2001 and Silver medal in 2009. He is a member of the editorial board of Indian Journal of Chemistry, Section B, Green Chemistry Task Force Committee, DST, Govt. of India and Chemrawn committee, IUPAC among others.

Invited Lectures

Designing a green reaction

Brindaban C Ranu
Department of Organic Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Kolkata – 700032, India
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ABSTRACT

The protection of environment is one of the major issues of this century and there is a growing concern on the use of environmentally friendly chemicals and materials. The toxic chemicals such as carbon tetrachloride, chloroform, phosgene and many other hazardous compounds are often used in chemical reactions and certainly, chemists have a significant role in the endeavor of greening of chemical processes and thus the environment. Thus, the concept of green or sustainable chemistry was originated in the early 1990 to reduce chemical related impact on human health and virtually eliminate contamination of the environment through dedicated, sustainable prevention programs. This philosophy gave impetus to the creation of a new way of thinking about chemistry and awareness of the need for innovative chemical technologies that accomplished pollution prevention in a scientifically sound manner. In classical organic reactions, the impact of reaction media, catalyst and generated waste on environment was largely ignored. Nevertheless, the use of large volumes of volatile hazardous organic solvents in industrial processes posed a serious threat to the environment as these constitute the major chemical waste. It is thus highly desirable to design reactions avoiding hazardous organic solvents, toxic catalysts and using safer chemicals. The primary parameters of designing a green reaction together with illustrative examples will be presented.

Invited Lectures

Dr. K. Avasthi

Scientist F
Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow-226001

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 (pi-pi) interactions. Design and Synthesis of bio-active molecules especially CNS/CVS active agents.

PUBLICATIONS 57

Reviews 2

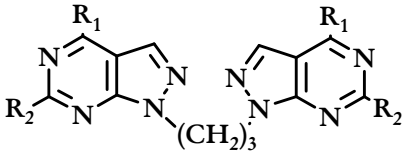
Invited Lectures

Pyrazolo[3,4-*d*]pyrimidine core as novel system for studying arene interactions in flexible polymethylene linker compounds especially propylene linker compounds

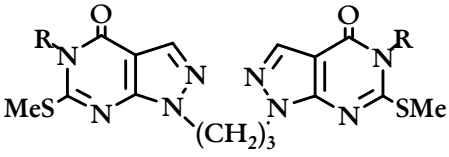
K. Avasthi
Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow-226001

ABSTRACT

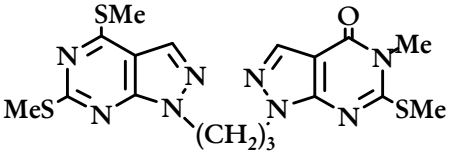
A new fully flexible model based on pyrazolo[3,4-*d*]pyrimidine (PP) core, which is isomeric with biologically important purine, for understanding of arene interactions in polymethylene linker compounds has been developed. During last fifteen years robustness of the model has been demonstrated in more than a dozen symmetrical (1 & 2)[1,2] and few dissymmetrical propylene linker compounds (3 & 4).[3] Importance of the position of propylene linker (1a vs. 5a) and substituent effect (6 & 7) on conformational control due to arene interactions in the model will be discussed. Application of such "protophanes" for the first synthesis of pyrazolo[3,4-*d*]pyrimidinophanes will be described.[4]



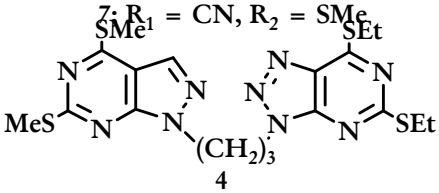
1a: R_1 = R_2 = SMe;
1b: R_1 = R_2 = SEt;
1c: R_1 = R_2 = S-iso-Pr;
1d: R_1 = OEt, R_2 = SMe;
1e: R_1 = O-isoPr, R_2 = SMe;
1f: R_1 = OMe, R_2 = SO_2Me;
1g: R_1 = OEt, R_2 = SO_2Me;
1h: R_1 = O-isoPr, R_2 = SO_2Me;
1i: R_1 = O-isoPr, R_2 = SO_2Et;
1j: R_1 = R_2 = OMe
6; R_1 = Cl, R_2 = SMe;
7; R_1 =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



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



3



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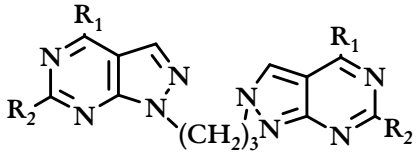

5a: R_1 = R_2 = SMe

Invited Lectures

Dr. Rakeshwar Bandichhor

Head, COE-Chemistry, R&D, Innovation Plaza Dr. Reddy's Laboratories
Hyderabad, India
E-mail: rakeshwarb@drreddys.com

Dr. Rakeshwar Bandichhor holds a doctorate in chemistry from University of Lucknow-University of Regensburg, Germany. He did his B. Sc. (Chemistry & Zoology) and his M. Sc. Tech. in Pharmaceutical chemistry from University of Lucknow.

Dr. Rakeshwar's previous professional experience includes working as Postdoctoral Fellow at University of Regensburg, Roy & Diana Vegelos Laboratories for Advanced Science & Technology, University of Pennsylvania and postdoctoral research associate at Department of Chemistry at Texas A&M University.

Dr. Rakeshwar has more than 80 papers including patents and book chapters published/accepted in various International Journals and another 14 papers submitted or under considerations.

He has won the various awards in his career e.g. Chairman Excellence Award in the category of individual functional excellence, Best Cost Leadership Award for the development of Lopinavir, Ritonavir & their components and Anveshan Award at Dr. Reddy's. He was also amongst the shortlisted candidates for Sir M. J. Collins Young Innovator Award. As a part of organizational building efforts, he also supervises master's & Ph.D. students in their dissertations. He has been invited in several conferences e.g. IIT-Mumbai, IGCW-2009, BIT-Ranchi, BITS Pilani, 9th Heterocyclic Conference, University of Florida, JNTU-Hyderabad etc. to deliver lectures.

Invited Lectures

Role of organic chemistry in healthcare: An industrial perspective

Rakeshwar bandichhor
Center of Excellence, Research & Development, Integrated Product Development, Dr. Reddy's Laboratories Ltd., Survey Nos. 42,45,46, & 54 Bachupally, Qutubullapur, Ranga Reddy Dist 500072, Andhra Pradesh, India
E-mail: rakeshwarb@drreddys.com

ABSTRACT

Since an onset of life which was scientifically proven by conducting an organic chemistry experiment. This experiment was designed by Miller and Urey[1] aiming to establish a fact that the origin of life was not from anywhere else but a chemical reaction that first afforded five amino acids. Reanalysis of original reaction mixture of Miller-Urey's experiment which was performed in 2008[2] in fact revealed that there were twenty amino acids synthesized in one single experiment proves the hypothesis of origin of life by chemical evolution. Moving on to mammalians' life that's where we belong to and it functions due to cascade of organic chemistry reactions catalyzed by myriad of enzymes. Right from birth to death our entire life is based on the chemical reactions that favour our existence. Understanding of the biochemical aspects of plants and animals bring a paradigm shift in discovery of several life saving medicines. Post discovery of the medicines, we are facing the problem of unavailability of affordable medicines today. Once again expertise in organic chemistry brings the solution by designing and practicing the robust, scalable and green synthetic routes for life saving medicines in a cost effective fashion. Few case studies as mentioned in the Figure 1 will be presented.

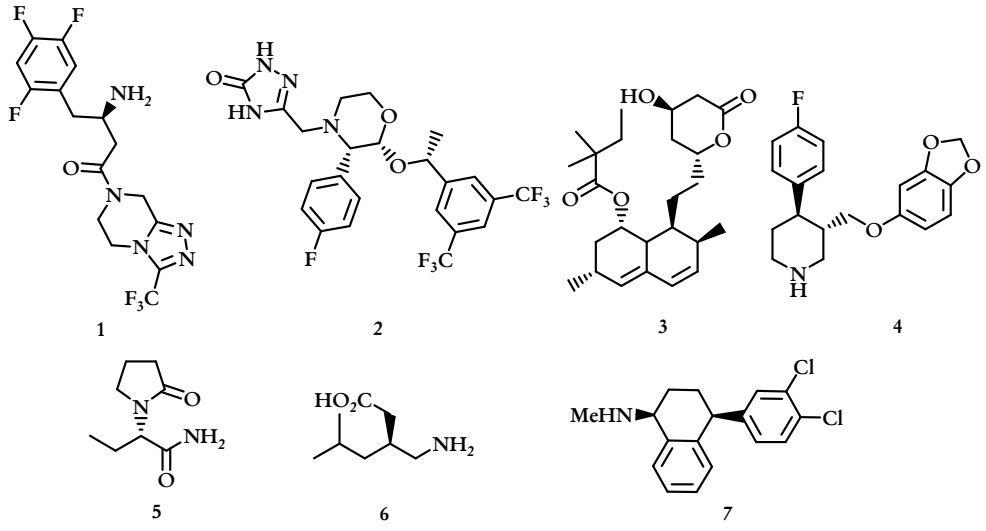

Figure 1: Few Drug Substances

Invited Lectures

Dr. Anjali M. Rahatgaonkar

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Novel approaches to synthesis of new nitrogen, oxygen & sulphur heterocycles with potential medicinal significance

Anjali M. Rahatgaonkar
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ABSTRACT

Nitrogen, oxygen & sulphur containing heterocycles are compounds with special synthetic interest not only because many of them are biologically active, but also because they posses different reaction centers which can be attacked by ambifunctional nucleophilic/electrophilic reagents. This property makes them attractive starting materials in medicinal chemistry as valuable building blocks for ring closure reactions to form mainly five, six and seven-membered heterocyclic compounds. Additionally, if α-methylene active hydrogen atoms with carbonyl functionality present in such compounds, it could open new possibilities for ring closure reaction and ring expansion. Herein we report the synthetic methods and ring expansion/closure reactions leading to synthesis of a library of nitrogen, oxygen & sulphur containing heterocycles. The novel and efficient methodology of synthesis of ring expansion of pyrimidines, isoxazoles, pyrazoles, thiazoles, thiazines, azetidinones, quinolines, flavonoids, coumarins etc is described in this review. The QSAR studies and significant medicinal properties of the all heterocyclic compounds are evaluated.

Invited Lectures

Dr. Nilesh M. Dagia

Piramal Research Centre, 1 Nirlon Complex, Goregaon (E), Mumbai -63, India
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E-mail: nilesh.dagia@piramal.com

SPECIALIZED SKILLS

- Mammalian cell culture
- Protein detection assays (e.g. ELISA)
- Multicolor flow cytometric analysis (FACS)
- Cell to cell flow adhesion and transmigration assays
- Blot-rolling assay
- Stamper-Woodruff assay
- Purification of human leukocytes from whole blood
- DNA transfection of mammalian cells
- Northern blot analysis
- Transcription activity analysis using luciferase assay
- Electrophoretic mobility gel shift assay
- Immunoprecipitation and Western blot analysis
- Reverse transcription polymerase chain reaction
- Mathematical modeling of biological systems
- Isolation of human hematopoietic stem cells from bone marrow, mobilized peripheral blood, and cord blood
- Isolation of cells from freshly harvested synovial tissue from patients with active disease
- In-vivo inflammation models (e.g., collagen-induced arthritis, adjuvant-induced arthritis, acute models of colitis, colitis-associated colon cancer, human psoriatic skin-SCID mice xenograft, experimental psoriasis, LPS-induced toxic shock, etc.)

AWARDS AND HONORS

- Editorial Board Member, *World Journal of Gastrointestinal Pathophysiology*
- Chief Guest, State Level Conference on "Recent Advances in Drug Delivery Systems", Seth Govind Raghunath Sable College of Pharmacy, Pune, India (2008)
- Inaugurated a national conference on "Current Scenario & Recent Advances in Cancer Therapy", Maharashtra Institute of Pharmacy, Pune, India (2008)
- Sponsorship for Invited Seminar, Diagnostic Hybrids Inc., Athens, OH (2005)
- Nominee, Council of Graduate Schools International Dissertation Award -Ohio University, Athens, OH (2004)
- Graduate Student Scholarship -Ohio University, Athens, OH (2000 -2004)
- Graduate Student Special Travel Award -Biomedical Engineering Society, Annual Fall Meeting (2002)
- First prize for project on "Scheduling and Simulation of Cement Mills" (2000)
- Graduated B.E with 6th rank (out of approximately 350 students) in Mumbai University (1999)

PROFESSIONAL MEMBERSHIPS (PAST and PRESENT)

- American Institute of Chemical Engineers (AIChE)
- Biomedical Engineering Society (BMES)
- Indian Institute of Chemical Engineers (IIChE)
- Omega Chi Epsilon, National Chemical Engineering Honor Society (OXE)
- Phi Kappa Phi, National Honor Society (PKP)

Invited Lectures

Dr. Navindra P. Seeram

Bioactive Botanical Research Laboratory, Department of Biomedical and Pharmaceutical Sciences, College of Pharmacy, University of Rhode Island, Kingston, RI, USA
E-mail: nseeram@uri.edu

Bioactive compounds from north american maple (*Acer*) species

Liya Li, Tao Yuan, Antonio Gonzales-Sarrias and Navindra P. Seeram*
Bioactive Botanical Research Laboratory, Department of Biomedical and Pharmaceutical Sciences, College of Pharmacy, University of Rhode Island, Kingston, RI, USA
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ABSTRACT

The maple (*Acer*) genus includes the sugar maple (*A. saccharum*) and red-leaf maple (*A. rubrum*) species which are endemic to North America. These maple species are the main source of maple syrup, a premium natural sweetener, which is obtained by boiling the sap collected from the trees. Phytochemical investigation of maple syrup and various plant parts resulted in the isolation and identification of more than 40 phenolic compounds several of which are new. The purified compounds, which included lignans, coumarins, stilbene and phenolic acid derivatives, as well as the maple plant extracts, showed antioxidant, anti-inflammatory and human cancer cell cytotoxicity activities. Therefore, these maple species should be further explored for their nutraceutical potential given their great abundance in North America.

ISCB Award for Excellence-2011 CHEMICAL SCIENCES

Prof.Katsuhiko Ariga

World Premier International (WPI) Research Center for Materials Nanoarchitectonics
National Institute for Materials Science
1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan
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E-mail: ARIGA.Katsuhiko@nims.go.jp

Major Fields

Supramolecular Chemistry, Surface Science, and Nanomaterials

Biography

1987-1992	Assistant Professor (Tokyo Institute of Technology)
1990	PhD (Polymer Science, Tokyo Institute of Technology)
1990-1992	Postdoctoral Researcher (University of Texas at Austin)
1992-1998	JST Group Leader (Supermolecules Project) and CREST Researcher
1998-2001	Associate Professor (Nara Institute of Science and Technology)
2001-2003	JST Group Leader (Nanospace Project)
2004-	Director of Supermolecules Group, NIMS
2007-	Principal Investigator, MANA, NIMS,
2008-	Visiting Professor (Tokyo University of Science)

Editorial Activity

Asian Editor of Journal of Nanoscience and Nanotechnology
Asian Editor of Advanced Science Letters
Asian Editor of Nanoscience and Nanotechnology Letters
Associate Editor of Physical Chemistry Chemical Physics
Associate Editor of Science and Technology of Advanced Materials
Associate Editor of *Chemistry Letters*
Editorial Advisory Board Member of *ACS Applied Materials & Interfaces*

Recent Research Activities on Supramolecular Materials

In our research, functional materials have been wisely constructed via bottom-up approaches as seen in preparation of molecular patterns and complexes, organized nanostructures, and function bulk materials. In addition, novel concepts "hand-operating nanotechnology" to bridge nano (molecular) structures and bulk systems is also initiated. These strategies enable us to construct hierarchic supramolecular structures, some of which are highly useful for bio-related applications such as drug delivery and sensing. Recently we have been developing microcapsules with mesoporous thin walls made from silica and carbon. For example, a novel hierarchic nanostructure based on layer-by-layer (LbL) assembly and mesoporous technology, so-called mesoporous silica nanocompartment film, was reported. The resulting films shows stimuli-free auto-modulated stepwise release of water or drug molecules. We also demonstrated the LbL assembly of various nanocarbon materials on a QCM plate and the use of the resulting structure for selective adsorption of gaseous substances. The related LbL structures of mesoporous carbons were demonstrated for in situ sensor use based on highly cooperative nanopore-filling adsorption in the liquid phase.

ISCB Award for Excellence-2011 CHEMICAL SCIENCES

Prof.Krishna Kumar

Chairman, Department of Chemistry,Tufts University, Medford, MA 02155
Telefon: +1 617 627 5651
Telefax: +1 617 627, 3443
E-mail: krishna.kumar@tufts.edu

Education

- The Scripps Research Institute and The Skaggs Institute for Chemical Biology, La Jolla, CA 92037
  Skaggs Research Fellow, Bioorganic Chemistry & Chemical Biology, June 1996-September 1998
- Brown University, Providence, RI 02912, Ph.D., *Organic Chemistry*, May 1996
- St. Stephen's College, University of Delhi, Delhi 110007, B.Sc. (Honours), *Chemistry*, May 1991

Research & Professional Appointments

2006-2009	Chairman, Department of Chemistry,Tufts University, Medford, MA
2007–present	Member, Cancer Center,Tufts Medical Center, Boston, MA 02110
2006-present	Professor of Chemistry,Tufts University, Medford, MA 02155
2004–2005	Visiting Scientist, Center for Cancer Research,Massachusetts Institute of Technology, Cambridge, MA 02138,(Professor Phillip A. Sharp, MIT Biology and CCR)
2003–2005	Associate Professor of Chemistry,Tufts University, Medford, MA 02155
2002–present	Adjunct Professor, Department of Biomedical Engineering, Tufts University School of Engineering, Medford, MA 02155
1999–2006	Associate Member, Cancer Center,Tufts–New England Medical Center, Boston, MA 02110
1998–2002	Assistant Professor of Chemistry,Tufts University, Medford, MA 02155

Awards and Affiliations

(1) Global Indus Technovator Award, MIT Indian Business Club, 2006
(2) Tufts Chemistry Faculty Achievement Award, Fall 2009
(3) Tufts Chemistry Faculty Achievement Award, Fall 2005
(4) DuPont Young Professor Award, 2003–2006

Research Activities

Krishna Kumar is Professor of Chemistry and Biomedical Engineering at Tufts University. After earning a B.Sc. with honors in Chemistry at St. Stephen's College in 1991, Kumar enrolled in the Department of Chemistry at Brown University, where he was awarded a Ph.D. in 1996 for work done under the supervision of Matthew Zimmt on long distance electron transfer mechanisms. Following postdoctoral work at the Scripps Research Institute in La Jolla, CA with M. Reza Ghadiri on self-replicating peptides, Kumar accepted an assistant professorship in the Department of Chemistry at Tufts University in the fall of 1998.

Kumar was promoted to Associate Professor (2003) and Professor (2006) at Tufts University in quick succession. He served as Chairman of the Department of Chemistry at Tufts from 2006 until 2009. He is a Member of the Cancer Center at the Tufts Medical Center in Boston. His research interests span synthetic organic chemistry, chemical biology, biophysics, and cell biology.

Kumar's contributions to science, and in particular chemistry, have been recognized widely. He was named a DuPont Young Professor, recognized as one of the top 35 young innovators in the world by MIT Technology Review magazine (TR35), awarded a Global Indus Technovator award from MIT-IBC, the National Science Foundation CAREER award, a Technology award from the Massachusetts Technology Transfer Center, and a BASF lectureship. He has received more than $ 6 million in research grants from various federal agencies in the US.

ISCB DISTINGUISHED WOMEN SCIENTISTS AWARD

Dr.(Mrs) Rukhsana I. Kureshy

Scientist – EII,
Central Salt and Marine Chemicals Research Institute (CSMCRI), Gijubhai Badheka Marg, Bhavnagar-364002, Gujarat (India)
Email: rukhsana93@yahoo.co.in

Field of Specialization

Chiral Metal complex based Asymmetric Catalysis under homogeneous and heterogeneous conditions.

Dr. Rukhsana I. Kureshy. M.Sc., Ph. D. Aligarh Muslim University, has research experience of 29 years with specialization in chiral catalysis. She has designed numerous chiral metal complexes and used them as efficient catalysts for various organic transformations such as asymmetric epoxidation, epoxide ring opening reaction and hydrolytic kinetic resolution of racemic terminal epoxides under homogeneous and heterogeneous systems. She has published more than 100 research papers in international journals and 6 patents to her credit. She was instrumental in developing a green catalytic process for the production of styrene oxide: an intermediate for perfumery chemical, which was eventually licensed for commercialization to two private industries. Her works were recognized through several awards that include, CSIR Young Scientist Award 1993, MAAS Best Paper Award 1993, Hari Om Ashram Prerit S. S. Bhatnagar Award 1996, MAAS Woman Scientist Award 2005 and MAAS Best Paper Award 2005. She is recognized Guide for Ph.D. from Bhavnagar University, Bhavnagar and several students have received Ph.D. degree under her guidance.

ISCB Young Scientist Award — CHEMICAL SCIENCES

Dr. Partha Sarathi Mukherjee

Inorganic & Physical Chemistry Department, Indian Institute of Science, Bangalore-560012;
E-mail: psm@ipc.iisc.ernet.in;
Homepage: http://ipc.iisc.ernet.in/psm.html

Present position

Associate Professor, Inorganic & Physical Chemistry Dept., Indian Institute of Science, Bangalore

Research fields

Supramolecular Chemistry, Magnetic and Organometallic Materials

Summary

• 12 years inorganic chemistry research in academia
• Practical knowledge of advanced synthetic and characterization methods
• 6 years teaching experience in chemistry at honours/PG level
• Co-author of 70 publications in peer-reviewed journals

Work Experience

2010-present	Associate Professor, Inorganic &Physical Chemistry Dept., Indian Institute of Science, Bangalore-560012.
2005-2010	Assistant Professor, Inorganic &Physical Chemistry Dept., Indian Institute of Science, Bangalore-560012.
2004-2005	Alexander von Humboldt Fellow at the Institute of Inorganic Chemistry, University of Goettingen, Germany. (Host: Prof. Herbert W. Roesky). Main group chemistry.
2003-05/2004	Post Doctoral Fellow, Department of Chemistry, University of Utah, USA. Supervisor: Prof. Peter J. Stang. Supramolecular chemistry and crystal engineering.

Significant contributions

My group has recently shown that predesigned organometallic nanoscopic cages with appropriate building blocks can be used to detect very trace amount of nitroaromatic explosives by fluorescence quenching method. Efficient sensors for the detection of explosives are high priority materials for security reasons in our country and in other south Asian countries.

ISCB Young Scientist Award BIOLOGICAL SCIENCES

Dr. Vikash Kumar Dubey

Associate Professor, Department of Biotechnology, Indian Institute of Technology Guwahati, Assam, India-781039
Tel: +91- 361-2582203, Fax: +91-361-2582249
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Born on May 1, 1975, Dr. Vikash Kumar Dubey received doctorate degrees from Banaras Hindu University, India. After his post-doctoral training at Florida State University, USA, he joined IIT Guwahati in 2006. Currently, Dr. Dubey is Associate Professor in Department of Biotechnology, IIT Guwahati. His research is focused on development of therapeutics against Leishmaniasis by targeting parasite specific metabolic pathways. Dr. Dubey has likewise made cutting edge contributions to the general knowledge of the scientific community regarding protein folding and the role of turn sequences in the stabilization of proteins. Moreover, Dr. Dubey has reported purification of novel proteases form a medicinal plant *Calotropis procera* and studied extensively with respect to activity-stability and folding. He has also been awarded DBT-Innovative Young Biotechnologist Award, Young Scientist Award of "The Biotech Research Society" and Young Scientist Award of "National Academy of Agricultural Sciences". He has authored about 40 peer-reviewed publications and 4 issued US patents. Indian Society of Chemists and Biologists is privileged to honour Dr Vikash Kumar Dubey with Young Scientist Award of the Society for his outstanding contributions in Biotechnology.

OL - 01

ORAL LECTURES

Novel saponins from the rhizomes of *Agapanthus africanus Linn.*

D. N. Singh* N. Verma and D. K. Kulshreshtha#
 # Scientist-G and Head (Rtd.), Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow-226001, India.
***Department of Chemistry, K. S. Saket PG College, Dr. RML Avadh University, Faizabad-224001, India.**
E-mail: dnsinghsaket@ yahoo.com

ABSTRACT

Plants continue to be an important source of generation of molecular diversity and compounds with unique pharmacological activity. There have been several breakthroughs recently including artemisinin from *Artemisia annua* for malaria, taxol from *Taxus baccata* for ovarian cancer, and gugulipid from *Commiphora wightii* for hyperlipidaemia. In the continuation of our work [1] to isolate and identify the plant constituents, recently we have isolated novel saponins from the n-butanol fraction of the rhizomes of *agapanthus africanus* (Liliaceae) a plant of south *African origin* [2,3] and the structures of the isolated saponins were established on the basis of their detailed chemical and spectral data (^{1}H NMR, ^{13}C NMR MASS, IR) analysis. In this paper, the details of the isolation procedure and characterizations of the isolated saponins will be discussed.

REFERENCES

[1] D. N. Singh, N. Verma, S. Raghuwanshi , P. K. Shukla and D. K. Kulshreshtha,; *Fitoterapia*,; 79, 2008, 298 .
[2] K. Takeda, Ann, Report Research Lab, 1955, Chem. Abstract, 50, 1956, 15916b.
[3] A.G. Gonzalez, R.Freire, C. G. Francisco, J.A. Salazar and E. Suarez. Phytochemistry, 13, 1974, 627.

OL - 02

ORAL LECTURES

Novel synthetic transformations employing carbon dioxide

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North-East Institute of Science and Technology (CSIR),
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ABSTRACT

Interesting synthetic elaborations have been accomplished employing carbon dioxide as cheap and safe alternatives for the incorporation of carbonyl functionality, eliminating use of harmful reagents such as carbon monoxide and phosgene.[1] Carbon dioxide has been frequently used in its various conditions and forms such as gaseous, electrochemical, supercritical and with various kinds of catalytic systems. In recent years, carbon dioxide has been frequently used as a cheap and safe alternative for the synthesis of carbamates,[2] carbonates[3] and several various other interesting organic transformations.[4]

In the present talk, I will focus various novel synthetic transformations employing gaseous carbon dioxide as a cheap and safe alternatives for the synthesis of carbamates, dialkyl carbonates, *O,S*-dialkyl carbonates (xanthates), *S*-alkyl carbamates, *S,S*-dialkyldithiocarbonates, carbazates and substituted ureas *etc.* starting from the diversity of starting materials.[5]

REFERENCES

[1] C B Dell'Amico, F Calderazzo, L Labella, F Marchetti, G Pampaloni, Chem Rev 103, 2003, 3857.
[2] **(a)** D Chaturvedi, et al. Curr. Org. Chem 11, 2007, 987; **(b)** D Chaturvedi, et. al. Curr. Org. Synth 4, 2007, 308.
[3] **(a)** A G Shaikh, S Sivaram, Chem. Rev 96, 1996, 951; **(b)** T Sakakura, K Kohno, Chem. Commun 2009, 1312.
[4] **(a)** H R Hobbs, N R Thomas, Chem Rev 107, 2007, 2786; **(b)** T Sakakura, J C Choi, H Yashuda, Chem. Rev 107, 2007, 2365.
[5] **(a)** D Chaturvedi, et al. Tetrahedron Lett 43, 2003, 7637; **(b)** D Chaturvedi, et al. Tetrahedron Lett 48, 2007, 5043; **(c)** D Chaturvedi, et al. Synthesis, 2008, 355; **(d)** D Chaturvedi, et al. Monatsh Chem 137, 2006, 201; **(e)** D Chaturvedi, et al. Monatsh. Chem 137, 2006, 459; **(f)** D Chaturvedi, et al. Monatsh Chem 139, 2008, 267; **(g)** D. Chaturvedi, et al. Synth Commun 26, 2002, *26,* 2651; **(h)** D. Chaturvedi, et al. Synth. Commun 38, 2008, 4013; **(i)** D. Chaturvedi, et al. J Iran Chem Soc. 2009, *6,* 510 ; **(j)** D Chaturvedi, et al. J Iran Chem Soc 7, 2010, 702.

OL - 03

ORAL LECTURES

Cellular internalization of water-soluble aromatic amide foldamers

J. Iriondo-Alberdi, K. Laxmi-Reddy, A. Bouguerne, C. Staedel, I. Huc*
Institut Européen de Chimie et Biologie, 2 rue Robert Escarpit, 33607 Pessac, France
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ABSTRACT

Intracellular transport of drugs and therapeutics represents one of the most exciting and challenging areas at the interface of chemistry, biology and medicine. Most of the effort in this field has so far been devoted to the development of peptide-based delivery systems that can translocate therapeutic agents into their intracellular targets.[1] More recently, the use of bio-inspired non-natural foldamers has resulted in the successful delivery of cargo molecules possessing a wide range of sizes and physico-chemical properties across the cell membrane.[2] We present here the synthesis of aromatic amide foldamers and their biological evaluation as cell-penetrating agents.[3] Using a well-established synthetic route, a series of fluorescein-labeled cationic aryl amide conjugates have been constructed and their cellular uptake into various human cell lines analyzed by flow cytometry and fluorescence microscopy. The assays have revealed that longer oligomers achieve greater cellular translocation, with the octamer proving to be a remarkable vehicle for all cell lines. Biological studies have also indicated that these helices are biocompatible, showing promise in their application as cell penetrating agents and as vehicles to deliver biologically active molecules into cells.

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OL - 04

ORAL LECTURES

3D QSAR study & pharmacophore identification and data mining for the current research trends of some substituted 2,3,4-trione-3-[(substituted phenyl)-hydrazones]

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ABSTRACT

Majority of the drugs in current use against Tuberculosis contains basic nitrogen, a lipophilic aromatic ring capable of interacting molecule at the drug receptor site. Our aim was to evaluate biological activity of a series of substituted 2,3,4-trione-3-[(substituted phenyl)-hydrazones] to identify common pharmacophore and develop atom based 3D QSAR model to get insights to find features which may be responsible for biological activity of these novel quinolone analogs for antitubercular activity. A highly predictive pharmacophore model was generated using a training set of 31 molecules which consist of two hydrogen bond donors, two hydrogen bond acceptor and two aromatic ring features. This six feature pharmacophore model can be used for virtual screening to discover more novel and potential molecules for the development of new anti-tubercular agents. Taking a step further, we researched for reported molecules with the similar chemical framework to explore other reported potential bioactivities. Further, we data mined and analysed the available published literature including patents to generate the substance landscape with their bioactivity indicators, current research trends etc.

OL - 05

ORAL LECTURES

Development of Vitamin E derivatives as anticancer agents

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ABSTRACT

Although, in the last two decades, we have witnessed tremendous development in molecular medicine, cancer still remains a major cause for mortality in developed countries. Moreover, due to heavy industrialization, developing countries like India and China are likely to be severely affected by cancer in coming decades. We are therefore in urgent need of anticancer agents that are efficient, selective and readily available. In recent advances, vitamin E derivatives have emerged as a novel group of selective anticancer agents. From their substation patterns, vitamin E derivatives can be divided into three domains such as (I) functional domain, (II) signaling domain and (III) hydrophobic domain (Figure 1). The most studied derivative of these VE analogs, ?-tocopheryl succinate (?-TOS, Figure 2), induces cancer cell death by disrupting mitochondria and causing the cytosolic release of modulator of apoptosis as well as by arresting the cell cycle in variety of cancer cells. In recent past, we have provided evidence that inhibition of BCL-xL/BcL-2 function represents a major pathway whereby ?-TOS mediates apoptosis induction in prostate cancer cells. More recently, we have reported a series of new vitamin E derivatives by the modification of hydrophobic domain and functional domain (Figure 3) which showed multi-fold improved anti-adhesion potency and anti-proliferative effects against various (MCF-7, SKBR3 and 4T1) tumor cell growths. Thus, the knowledge of structure-function relationship of VE derivatives will provide a base for further optimization of new VE analogs. In this context, a brief summery of the importance of all three domains of VE derivatives (structure-function study) for their anticancer activity will be presented.

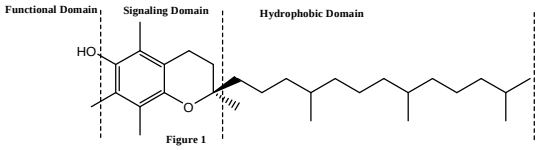

Figure 1

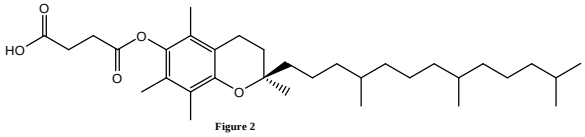

Figure 2

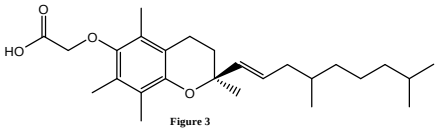

Figure 3

OL - 06

ORAL LECTURES

Characterization of potential phosphate dissolving bacterial culture isolated from sugar cane rhizosphere

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ABSTRACT

Phosphorus is the second important plant nutrient after nitrogen Donahue et al [1]. Phosphorus availability is low in soils because of its fixation as insoluble phosphates of iron, aluminum and calcium. Phosphorus supply through biological means is a viable alternative; phosphate solubilizing microorganisms (PSM) are active in conversion of insoluble phosphate to soluble primary and secondary orthophosphate ions Gyaneshwar et al [2]. Numerous microorganisms, especially those associated with roots have the ability to increase plant growth and productivity Chang et al [3]. Phosphate solubilizing bacterium isolated from sugar cane rhizospheres Chakkarvarthy et al [4] as SVM 18 was characterized in the present research work. Potential use of this bacterium as bioinoculant depends exclusively on growth conditions. Its physiological and biochemical characterization was done by various methods like soluble phosphorus estimation M L Jackson [5], phosphatase estimation Bhattacharjee et al[6], growth curve, effect of P^H, temperature and salt concentration on growth, different biochemical characterization, and antibiogram studies as well as determination of N_2 fixing abilities. Biochemical characterization was also done using GC-MS Sharif et al. [7] and API. Isolated culture has good potential as phosphatic biofertilizer.

OL - 07

ORAL LECTURES

Polyethylene glycol (PEG) as an efficient recyclable medium for the One-pot synthesis of 2,4,5-triaryl imidazoles

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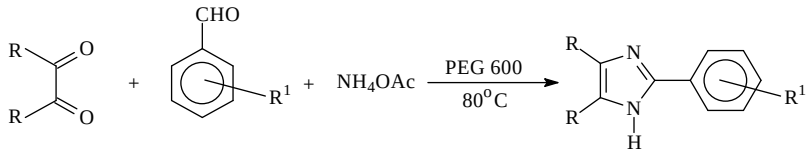
ABSTRACT

Organic reactions without the use of harmful organic solvents are of great interest in the development of synthetic methods Anastas et al [1]. Compounds with imidazole ring system have many biochemical Maier et al [2] and chemical Hermann et al [3] properties. There are several methods reported in literature for the synthesis of imidazoles such as reaction of N-(2-oxo)-amides with ammonium trifluroacetate Claiborne et al [4], 1,2-aminoalcohols in the presence of PCl_5 Bleicher et al [5], diketones, aldehyde, amine and ammonium acetate in phosphoric acid Liu et al [6], in acetic acid Sarshar et al [7]. Recently, combinations of the supported reagents and micro-wave (MW) irradiation such as MW/silica gel Balalaie et al [8], MW/Al_2O_3 Usyantinsky et al[9], MW/Acetic acid Wolkenberg et al [10] were used to carry out the synthesis of 2,4,5-triaryl imidazoles. More recently, 2,4,5-triaryl imidazoles were prepared from the reaction of aldehyde, 1,2-diketone or α-hydroxyketone and ammonium acetate in room temperature ionic liquid [Hbim]BF_4 at 100°C with good yields Srinivason et al [11]. Polyethylene glycol (PEG), a biologically acceptable polymer has hitherto not been widely used as a solvent medium but has been used as a support for various transformations Dickerson et al [12]. In continuation with our research on the development of novel synthetic methods Bandgar et al [13], we report here an efficient one-pot condensation of 1,2-diketone, aromatic aldehyde and ammonium acetate in the PEG-600 at 80°C which afforded 2,4,5-triaryl imidazole derivatives in excellent yields (Scheme 1).



1 2 3 4

Scheme 1

OL - 08

ORAL LECTURES

Structure activity relationship (SAR): Synthesis of new non steroidal anti inflammatory drugs (NSAIDs) considering diclofenac as a lead compound

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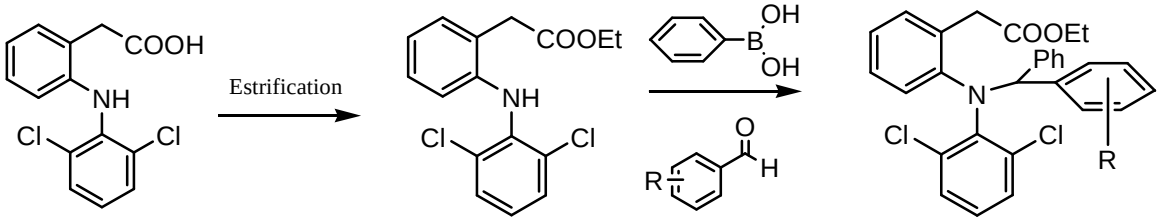
ABSTRACT

Structure-activity relationships (SAR)[1] are the traditional practices of medicinal chemistry which try to modify the effect or the potency (i.e. activity) of bioactive chemical compounds by modifying their chemical structure. Medicinal chemists use the techniques of chemical synthesis to insert new chemical groups into the biomedical compound and test the modifications for their biological effects. Diclofenac is a nonsteroidal anti-inflammatory drug (NSAIDs) that is effective for treating the fever, pain, and swelling caused by inflammation.. Other members of the NSAID class of drugs[2,3] include Fenoprofen, Ketoprofen, Indomethacin (Indocin), nabumetone (Relafen), naproxen (Aleve) and several others.By following a synthetic scheme [4] mentioned below, Diclofenac structure is modified by replacing hydrogen of Secondary amine by various aryl groups . In this way various new analogs of Diclofenac are synthesized. Further, all these analogs are esters, which will act as pro drugs [5] to be metabolized in vivo into active metabolites.



R= H, -CH_3,-OMe,-Cl , -NO_2

Scheme

OL - 09

ORAL LECTURES

Preclinical development of a novel triptolide prodrug for pancreatic cancer

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ABSTRACT

Pancreatic cancer is a particularly aggressive and devastating disease with a five-year survival rate of less than 5%. No effective drug treatment is currently available which can effectively prolong patient survival and efforts are urgently needed to develop innovative and effective treatments. Resistance to chemotherapy is a key factor preventing response to therapies in pancreatic cancer patients. Heat shock protein 70 (Hsp70) is known to be upregulated and over-expressed in pancreatic cancer cells as compared to normal cells. Furthermore, HSP70 has a protective effect on cancer cells inhibiting apoptosis of the cells. Inhibition of HSP70 in pancreatic cancer cells has been shown to increase apoptotic cell death. Triptolide, a naturally occurring compound obtained from the plant *Tripterygium wilfordii*, inhibits HSP70 expression and results in apoptotic cell death and inhibition of tumor growth *in vivo*. In addition, Triptolide inhibits nuclear factor kappa beta (NFkb), which also affords protection against apoptosis in cancer cells. These effects of triptolide are a very exciting finding with great therapeutic potential. While triptolide is very effective in inducing cell death in pancreatic cancer cells, its limited solubility and poor bioavailability limits its usefulness in the clinical scenario. The goal of this research is to prepare a novel triptolide prodrug with improved aqueous solubility that can be used for *i.v.* and oral administration. Here we present the design, synthesis and *in vitro* and *in vivo* evalution of a novel triptolide prodrug. This novel prodrug is a stable, soluble prodrug form of triptolide which provided dramatically improved aqueous solubility compared to the parent molecule, demonstrated rapid enzyme-mediated cleavage *in vitro*, effectively inhibited pancreatic cancer cell growth *in vitro* and inhibited cancer tumor growth *in vivo*. A phase I clinical trial of this novel triptolide prodrug is planned.

ORAL LECTURES

β-Oxodithioesters as versatile synthons in multicomponent reactions

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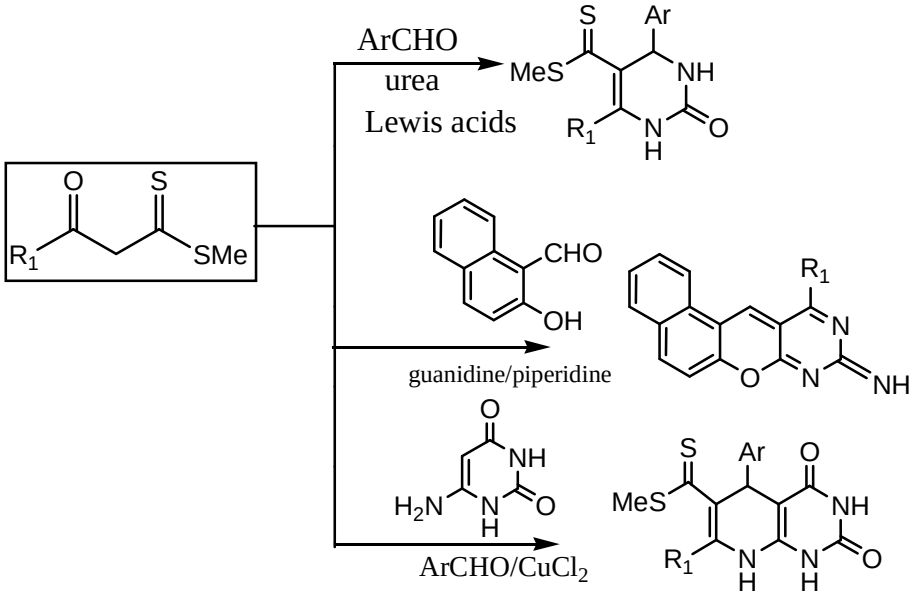
ABSTRACT

β-Oxodithioesters[1] 1 have been shown to be valuable synthetic intermediates in a variety of transformations leading to bioactive heterocycles. In continuation of our studies on the multicomponent reactions and β-Oxodithioesters,[2] we are disclosing herewith further multicomponent reactions using these intermediates to yield the diverse heterocyclic frameworks as shown in the following scheme.



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OL - 11

ORAL LECTURES

Click chemistry guided synthesis of 1,4-substituted triazoles as Src kinase inhibitors

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ABSTRACT

A protein kinase is an enzyme that modifies other proteins by chemically adding γ-phosphate group from ATP to them. Protein phosphorylation regulates most aspects of cell life, whereas abnormal phosphorylation can result devastating human diseases including cancer, chronic inflammation and diabetes. Src family kinases have important roles in the regulation of a wide variety of normal cellular signal transduction pathways. Src tyrosine kinase expression is frequently elevated in a number of epithelial tumors including colon, breast, prostate, lung, ovary and pancreas compared with the adjacent normal tissues. Therefore, development of Src kinase inhibitors has became a subject of major interest.[1] In recent years, "click chemistry" has become a very popular topic in drug discovery, bioconjugation due to the high reaction yield and simple reaction and purification conditions.[2] In our search for new Src kinase inhibitors[3] we became interested in the application of click chemistry reaction to design and identify novel Src kinase inhibitors. Our first approach involves functionalisation of pyrazolo[3,4-*d*]pyrimidines at N_1 position with differently substituted triazole rings using click reaction. In our second approach we designed and synthesized two seies of β-keto-1,2,3-triazoles. All compounds were evaluated for inhibition of Src kinase. Pyrazolo[3,4-*d*]pyrimidine triazoles exhibited good inhibitory potency (IC_{50} = 5.6-9.1 μM) against Src kinase whereas β-keto-1,2,3-triazoles showed modest inhibition of Src kinase. The details of synthesis and Src kinase inhibitory activities of these novel triazole derivatives will be presented.

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OL - 12

ORAL LECTURES

Chemistry methodologies and how technology can help improve productivity in the 21st century!

Dr. Omar Jina, Syrris Ltd, U.K.

ABSTRACT

"Practical Organic Chemistry has been performed in a largely similar way for over 100 years. There have been significant investments made in North America, Europe and Japan since the early 1990's in the automation of Chemistry, but these investments have not always demonstrated success in improving output. An increasing range of approaches have started to gain significantly more success since 2000. This is a review of some of the history of success and failure, as well as a look at some of the latest tools and technologies relating to the automation of practical chemistry, Flow Chemistry and software to help make better decisions in research projects".

PP - 001

Poster Presentations

Synthesis and biological evaluation of 4-styrylcoumarin derivatives as inhibitors of TNF-α and IL-6 with anti-tubercular activity

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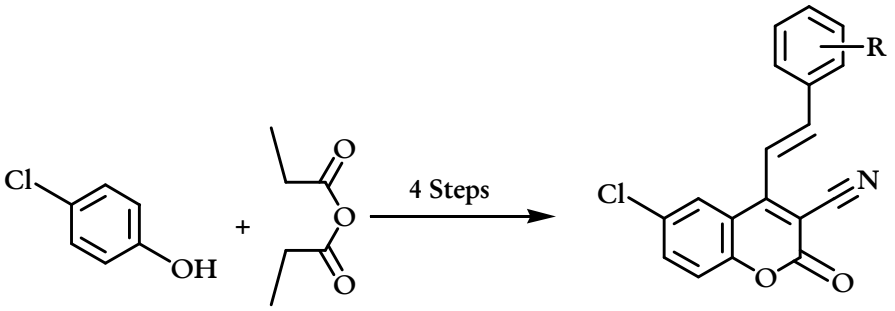
ABSTRACT

A series of 4-Styrylcoumarin have been synthesized by knovengle condensation between substituted 4-methylcoumarin-3-carbonitrile and different heterocyclic or aromatic aldehydes. 4-methylcoumarin-3-carbonitrile has been synthesized by the base catalysed reaction between substituted 2-Hydroxyacetophenone and ethyl cyanoacetate. The structures of the newly synthesized compounds were confirmed by 1H NMR, IR and Mass spectral analysis. All the compounds were evaluated for their anti-inflammatory activity (against TNF-α and IL-6) and anti-tubercular activity. Compounds 6a, 6b, 6h and 6j exhibited promising activity against IL-6 with 72–87% inhibition and compound 6v showed potent activity against TNF-α with 73% inhibition at 10 μM concentration. Whereas compounds 6n, 6o, 6r and 6u showed very good anti-tubercular activity against *Micobacterium tuberculosis* H37Rv strain at $<6.25\mu$M.



6-chloro-2-oxo-4-[-2-sub.ethenyl]-2*H*-chromene-3-carbonitriles

22 examples

R = substituted phenyl ring

PP - 002

Poster Presentations

A simple and efficient synthesis of pyrano chromene derivatives as potent anti HIV agents

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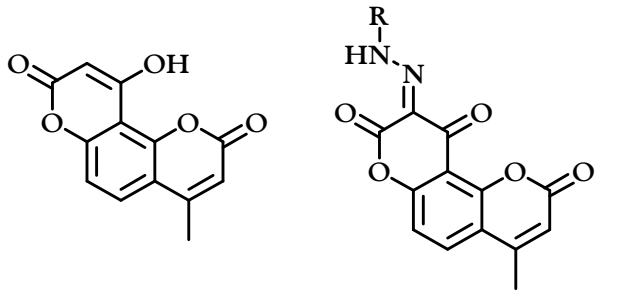
ABSTRACT

Chromenes are structurally simple compounds belonging to a large class of molecules known as benzopyrans and chroman-4-one moiety is an integral part of many natural products. These compounds and related derivatives have diverse biological activities, including antitumor, bacteriostatic that makes these compounds attractive for further backbone derivatization and screening as a novel therapeutic agent.[1-3] Chroman-4-one derivatives have also drawn much attention due to their HIV-1 activity.[4] Here in we reported a simple and practical synthesis of pyrano chromene derivatives and their biological activity.



R = 4-NO2-Ph, 2-Cl-Ph, 2-OH- Ph

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PP - 003

Poster Presentations

3D- QSAR study of 1,4-dihydropyridine derivatives for tumour-specific cytotoxicity

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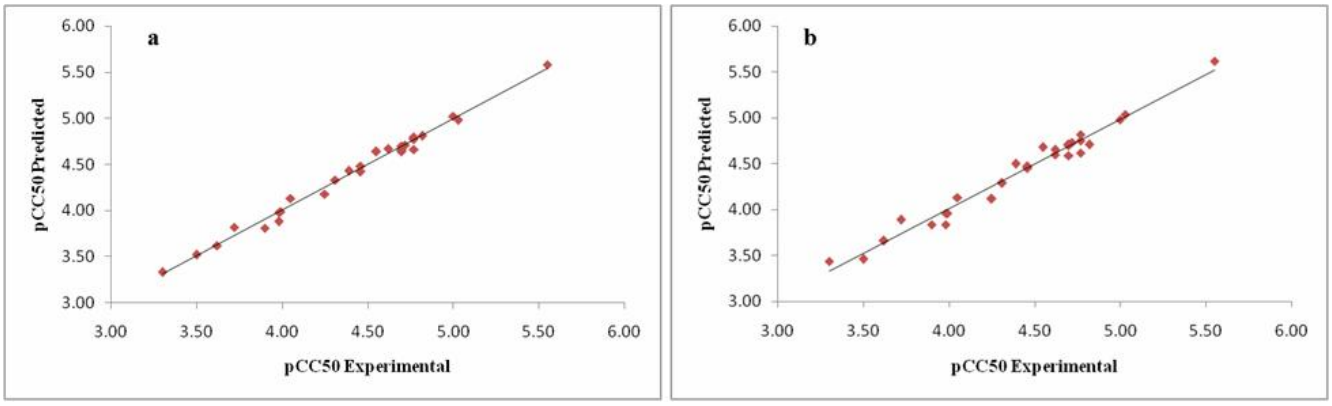
ABSTRACT

The 3D-QSAR analysis of 1,4-diphenyl-1,4-dihydropyridine and other 1,4-dihydropyridine derivatives were carried out. A set of 35 compounds were synthesized and evaluated for their cytotoxic activity in human cancer cell line HL-60. In order to establish relationship between structure and biological activity, 3D-QSAR study has been carried out using comparative molecular field analysis (CoMFA) and Comparative Molecular Similarity Indices Analysis (CoMSIA) using atom-fit alignment strategies. Among several generated models, database alignment based model was the best in terms of overall statistics with correlation coefficient (r^2) of 0.989 and 0.974 respectively and cross validated correlation coefficient (q^2) of 0.65 and 0.69 respectively.



Plots of actual *versus* predicted pIC_{50} values of training set molecules (a) CoMFA (b) CoMSIA

PP - 004

Poster Presentations

DNA-directed alkylating agents: Synthesis and antitumor activity of phenyl *N*-mustard-quinazoline conjugates having a urea linker

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ABSTRACT

Designing DNA-directed alkylating agents is one of the more effective strategies to overcome the general drawbacks of DNA alkylating agents. Recently, we utilized quinolines as carriers to prepare a series of *N*-mustard-quinoline conjugates having a urea or hydrazinecarboxamide linker. These conjugates possess potent antitumor activity against a variety of human tumor cell growth *in vitro*. To continue our research on developing new DNA-directed alkylating agents as potential anticancer agents, we synthesized a series of *N*-mustard-4-anilinoquinazoline conjugates bearing a urea linker at C-6 position for antitumor evaluation. Various substituent(s) was introduced to the C-4 anilino moiety for study the structure-activity relationships of these conjugates. The antitumor studies revealed that these agents exhibited significant antitumor activity in inhibiting various human tumor cell growths in culture. The therapeutic efficacy of selected compounds against human breast carcinoma MX-1 and prostate PC-3 xenograft in animal model were studied. These agents showed 54–75% tumor suppression with low toxicity (5–7% body-weight changes). We also demonstrate that the newly synthesized compounds are able to induce DNA cross-linking through alkaline agarose gel shift assay and inhibited cell cycle arrest at G2/M phase. The chemical synthesis as well as antitumor activity of these conjugates will be presented.

PP - 005

Poster Presentations

Simple and efficient cleavage of *N*-BOC group using SiO_2 under microwave irradiation

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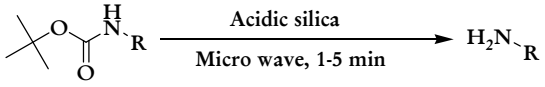
ABSTRACT

A facile and rapid method have been developed for the removal of N-Boc protecting groups using Silica under Microwave irradiation to regenerate the parent amine in high yields. The reaction is heterogeneous in nature and afforded pure amine without basification. The silica can easily be removed by simple filtration and then solvent was evaporated to give final compound. In addition, silica was recovered and utilize again.



PP - 006

Microwave assisted N-alkylation of 2-methyl indoline and isatin derivatives as antimicrobial agent

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ABSTRACT

A simple and an efficient Microwave Assisted N-alkylation have been demonstrated. Herein we reported the reaction of 2-methyl indoline /Isatin with halo alkylating agent in the presence of base and DMF as catalyst. The present method has advantages over the conventional method by means of lesser reaction time, easy work up and higher yield with better purity. The synthesized compounds were screened for the antimicrobial activity against four strains and have moderate to potent activity against all four strains.

PP - 007

Poster Presentations

Synthesis and in vitro antitubercular activity of 1,4-dihydropyridine

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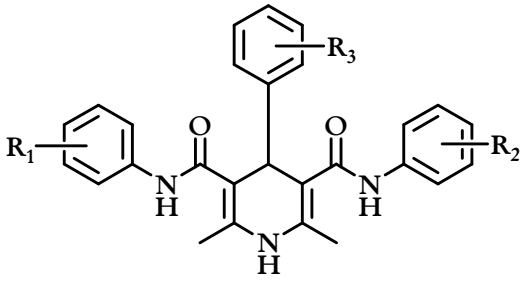
ABSTRACT

1,4-Dihydropyridines represent a very important class of heterocyclic moiety. The 1,4-dihydropyridines possess wide range of biological activities. Present work reports the synthesis of symmetric 1,4-dihydropyridines. Compounds were synthesized following Hantzch Synthesis using substituted acetoacetanilide, arylaldehydes and ammonia. Newly synthesized compounds were confirmed by ^{1}H NMR, ^{13}C NMR, Mass and IR spectral analysis. 1,4-dihydropyridine derivatives were tested for their activity against *M. tuberculosis* H37Rv strain with rifampin as the standard drug. Compounds 1,2,18 and 19 exhibited promising activity with the percentage inhibition of 93%, 92%, 85% and 77% respectively.



Subdtituted 1,4-dihydropyridine
20 examples

Where
$R_1 = R_2 = CH_3$, OCH_3, NO_2, Cl, CF_3
$R_3 = OCH_3$, OH, NO_2, Cl, Br, etc

PP - 008

Poster Presentations

Development and validation of a reversed-phase ultra-performance liquid chromatographic method for the simultaneous determination of six drugs used for combined hypertension therapy

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ABSTRACT

An isocratic, simple, rapid and reliable ultra performance liquid chromatographic assay method has been developed for the simultaneous estimation of orally administered hypertension drugs (atenolol, hydrochlorothiazide, amlodipine besylate, indapamide, nifedipine and lercanidipine hydrochloride) of which atenolol is administered with anyone of the other five drugs in combined hypertension therapy. Chromatography was carried out at 25°C on a 2.1 × 50 mm i.d., 1.7 μm Acquity BEH C_{18} column with the isocratic mobile phase of 0.01 M, 4.0 pH, aqueous phosphate buffer and acetonitrile (50:50, v/v) at a flow rate of 0.35 mL/min. All drugs were separated in less than 4 min with good resolution and minimal tailing, without interference of excipients. The method was validated according to ICH guidelines and the acceptance criteria for accuracy, precision, linearity, specificity and system suitability were met in all case. The column effluent was monitored at 230 nm. The detector response was linear in the range of 1-20 μg/mL of these drugs. Limit of detection obtained were 0.04 μg/mL for atenolol, 0.02 μg/mL for hydrochlorothiazide, 0.03 μg/mL for amlodipine besylate, 0.03 μg/mL for indapamide, 0.02 μg/mL for nifedipine and 0.01 μg/mL for lercanidipine hydrochloride. The suggested method has advantage that all the drugs can be quantified alone or in combination with atenolol using single mobile phase.

PP - 009

Poster Presentations

Utilization of quinoline derivative synthesized via microwave assisted one-pot protocol

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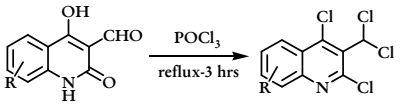
ABSTRACT

Quinoline moiety has great importance in synthesis of variety of drug. Quinoline itself contains variety of biological activity. Herein we have developed a short, efficient and simple one-pot microwave as well as conventional process for the preparation of small library of 2,4-dihydroxy quinolines, followed by Riemer-Tiemann Formylation to afford 3-fornyl-4-hydroxy-2-quinolone. Nucleophilic chlorination of 4-hydroxy-3-formyl-2-quinolione derivatives with phosphorus oxychloride was afforded 2,4-dichloro-3-(dichloromethyl) quinolines in high yields for further synthetic as well as biological interest.



R= -CH_3, -OCH_3, -X, -NO_2, etc.

PP - 010

Synthesis and antimicrobial activity of 1-(aroyl / arylsulpho) aminoindane

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ABSTRACT

1 – Aroyl aminoindane (2a – 2j) and 1 – arylsulphonamidoindane (3a – 3j) have been synthesized. The products have been assayed for their biological activity against Gram +ve, Gram –ve bacteria and fungi. Some of the products showed moderate activity in concentration 50 μg/ml. The structures of the products have been elucidated by IR, ^{1}HNMR, Mass spectral data and elemental analysis.

PP - 011

Poster Presentations

Water mediated construction of methyl 4-methyl-1*H*-benzimidazole-6-carboxylates using etidronic acid as catalyst

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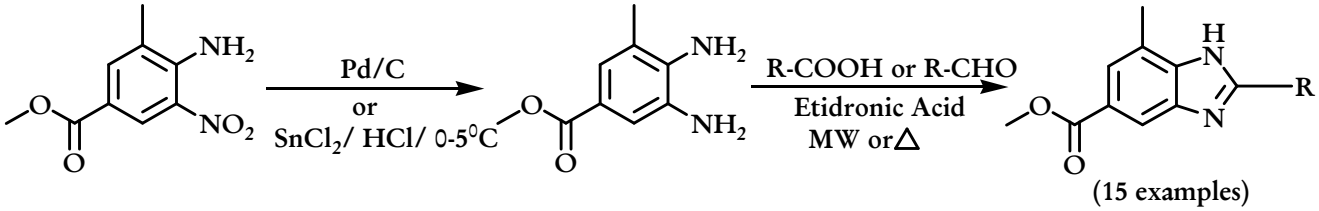
ABSTRACT

Benzimidazoles are characterized as privileged structures in medicinal chemistry because of their ability to interact with a range of different enzymes and receptors. Present work reports the water mediated, Etidronic Acid catalysed synthesis of methyl 4-methyl-1H-benzimidazole-6-carboxylates. Cyclization of methyl 3,4-diamino-5-methylbenzoate with substituted carboxylic acids or aldehydes proceeds in both conventional as well as Microwave assisted reaction environment. Newly synthesized compounds were confirmed by ^{1}H NMR, ^{13}C NMR, Mass, and IR spectral analysis.



R = -CH_3, -CF_3, -C_6H_5, -p-ClC_6H_4, -o-OHC_6H_4, -C_5H_4N, etc.

PP - 012

Poster Presentations

Ultra performance liquid chromatographic method for simultaneous determination of nine most pertinent antipsychotic molecules

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ABSTRACT

A selective Ultra Performance Liquid Chromatographic (UPLC) method for the simultaneous determination of nine most pertinent antipsychotic molecules has been developed, which includes Venlafaxine, Escitalopram, Fluoxetine, Candesartan, Risperidone, Trihexyphenidyl, Thioridazine, Aripiprazole and Trifluoperazine. The method includes Reversed Phase Acquity™ BEH C_{18} column (50 mm × 2.1 mm i.d. and 1.7μ particle size). The mobile phase consists of acetonitrile and 10 mM ammonium Acetate with gradient elution. The flow rate was 0.3 ml/min and UV detection was performed at 215 nm. A System Suitability Test (SST) was developed to govern the quality of the separation. The developed method has been validated further with respect to Linearity, Accuracy, Precision, Selectivity, LOD, LOQ and Robustness. Different batches of samples were examined using this method. Furthermore, the method has proven to be successful when applied to analyze marketed pharmaceutical dosage formulations.

PP - 013

Synthesis and *in vitro* pharmacological studies of some novel 6-haloquinazolin-4(3*H*)-ones bearing pyrazole moiety

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ABSTRACT

A new series of pharmacologically important 2-[(2-phenyl)amino] phenyl methyl -3-[(1-phenyl-5-substituted phenyl)-1-hydro-1*H*-pyrazol-3-yl-amino]- 6-iodoquinazolin-4(3*H*) ones $D_{1\text{-}13}$ have been synthesized by the condensation of 2-[(2-phenyl)amino]phenyl methyl -3-[(substituted phenyl)]chromen amido-6-iodoquinazolin-4(3*H*)ones with phenyl hydrazine in the presence of glacial acetic acid. The compound 2-[(2-phenyl) amino] phenyl methyl-3-acetamido-6-iodo quinazolin-4(3*H*) ones B were synthesized from 3-amino-2-[(2-phenyl) amino] phenyl methyl-6-iodoquinazolin-4(3*H*) one A on treatment with acetyl chloride followed by condensation with different substituted aromatic aldehyde 2-[(2-phenyl)amino]phenyl methyl -3-[(substituted phenyl)]chromen amido-6-iodoquinazolin-4(3*H*)ones $C_{1\text{-}13}$ were obtained which on treatment with phenyl hydrazine in the presence of glacial acetic acid afforded title compound. The structures of newly synthesized compounds are established by IR, ^{1}H NMR, ^{13}C NMR and elemental analysis. The *in vitro* antibacterial and antifungal activity of synthesized compounds have been evaluated by cup-plate method.

PP - 014

Poster Presentations

Synthesis and biological activity of potent bifunctional DNA alkylating agents, pyrrolo[1,2-*b*]isoquinoline derivatives

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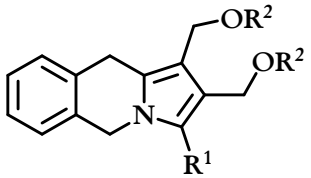
ABSTRACT

The naturally occurring antitumor Mitomycin C (MMC), which possess two reactive nucleophilic centers are capable of cross-linking with DNA. The other synthetic antitumor bifunctional alkylating agents, bis(hydroxymethyl)pyrrolizines derivatives were also able to induce DNA cross-linking via a similar mechanism of action of MMC. Based on the mechanism of action of these agents, we recently reported a series bis(hydroxymethyl)-8*H*-3a-azacyclopenta[*a*]indene-1-yl and their bis(methylcarbamates) derivatives. These derivatives were shown to have potent anticancer activity against various solid tumors cell growths in vitro and in vivo xenografts. To find new DNA bifunctional alkylating agents, we recently designed and synthesized a series of bis(hydroxymethyl)pyrrolo[1,2-*b*]isoquinolines and their bis(alkylcarbamate) derivatives for antitumor studies. These agents were found to have significant cytotoxicity against human leukemia (CCRF-CEM) and various tumor cells growth in vitro. The selected compounds were evaluated for their therapeutic efficacy in nude mice bearing human tumor xenografts. Complete tumor remission in nude mice bearing human breast (MX-1) xenograft and significant suppression in ovarian (SK-OV-3) xenografts were observed in animal models. The mechanism of action study demonstrated that these agents are able to cross-link with DNA by agarose gel shifting assay and induce cell arrest at G2/M phase. The chemical synthesis and antitumor activity of these derivatives will be presented.



R^1 = Alkyl or substituted phenyl
R^2 = H, CONHMe, CONHEt, CONH-*i*-Pr

PP - 015

Poster Presentations

An efficient and rapid synthesis of highly functionalized novel symmetric 1,4-dihydropyridines using glacial acetic acid as solvent

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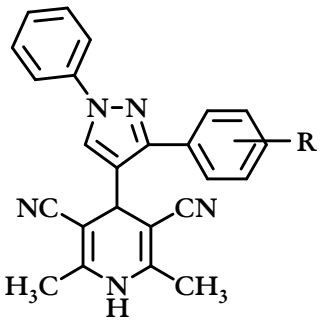
ABSTRACT

A series of 1,4-dihydropyridines bearing a pyrazole moiety in 4-position were synthesized by a variation from the classical Hantzsch synthesis. The reaction of 1,3-diphenyl-1*H*-pyrazole-4-carbaldehyde with 3-amino crotononitrile in the presence of glacial acetic acid afforded novel 3,5-dicyano 2,6-dimethyl 1,4-dihydropyridines. The main advantage of the procedure is short reaction time (15-20 min), easy workup procedure and high yield of novel dicyano, dimethyl and pyrazole substituted dihydropyridines.



Where R = H, CH_3, OCH_3,Cl, F etc..

PP - 016

Poster Presentations

Microwave assisted novel benzofuran-2-yl(4,5-dihyro-3,5-substituted diphenylpyrazol-1-yl) methanones and *in vitro* anticancer screening against MDR reversal cell line

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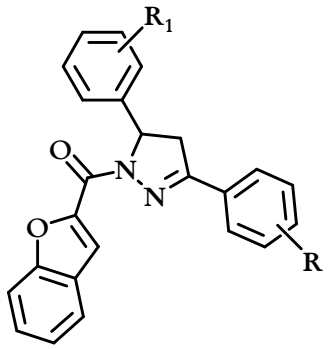
ABSTRACT

Microwave assisted synthesis of benzofuran-2-yl(4,5-diydro-3,5-substituted diphenylpyrazol-1-yl)methanone derivatives by the reaction of the benzofuran-2-carbohydrazides with various chalcone derivatives has been reported. The main advantage of the process is easy workup process, short reaction time and high yield of the new compounds for biological interest, the synthesized benzofuran derivatives were studied against human cancer cell lines for their antiproliferative activity and reversal of multidrug resistance on human MDR1 gene transfected mouse lymphoma cells.



where R = H, 4-Cl, 4-F.
R_1 = H,4-CH_3,4-NO_2 etc.

PP - 017

Poster Presentations

Development and validation of eight antihypertensive drugs in pharmaceutical products by UPLC-PDA

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ABSTRACT

An UPLC-PDA method was developed and validated for the simultaneous quantitative determination of diltiazem, quinapril, Valsartan, candesartan, carvedilol, olmesartan, ranolazine and Losartan for the determination of compounds in pharmaceutical products. The separation was achieved on Acquity UPLC BEH C8 (100mm X 2.1mm, 1.7μm, Waters) column by use of a mobile phase consisting of 0.2% Formic acid aqueous solution and acetonitrile 13 min. All calibration curves were linear (R^2=0.9990) over the tested ranges. The linearity ranges were 42.56 to 191.52 μgmL^{-1} for diltiazem, 40.64 to 182.88 μgmL^{-1} for quinapril, 41.92 to 188.64 μgmL^{-1} for Valsartan, 40.00 to 180.00 μgmL^{-1} for candesartan, 40.32 to 181.44 μgmL^{-1} for carvedilol, 44.16 to 198.72 μgmL^{-1} for olmesartan, 40.96 to 184.32 μgmL^{-1} for ranolazine and 43.20 to 194.40 μgmL^{-1} for Losartan. The method was validated by determining its sensisitivity, linearity, accuracy and precision. The purposed method is simple, fast, Linear, accurate, rugged and precise and hence can be applied for the determination of diltiazem, quinapril, Valsartan, candesartan, carvedilol, olmesartan, ranolazine and Losartan. The result show that the procedure is suitable for the routine analysis of drug.

PP - 018

Synthesis and anti-bacterial activity of poly-substituted pyrrole derivatives

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[1]Department of Chemistry, Saurashtra University, Rajkot.
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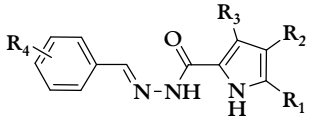
ABSTRACT

Organic compounds possessing nitrogen containing five membered heterocyclic rings are widely distributed in nature and often play an important role in various biochemical processes. Nitrogen containing heterocycles are subunits found in numerous natural products and in many biological active pharmaceuticals. Therefore, here in we have reported easy and efficient synthesis of poly-substituted pyrrole via condensation of α-amino ß-keto esters with acetyl acetone and their anti-bacterial activity.



PP - 019

Poster Presentations

Synthesis of acetyl pyrazolines & cyanopyridines via functionalization of chalcones

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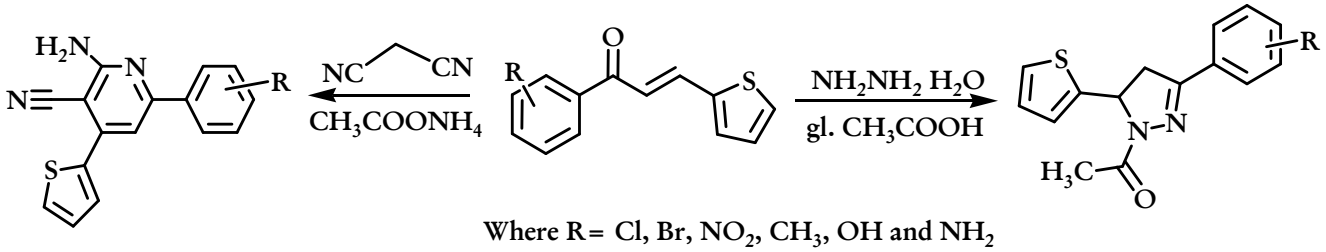
ABSTRACT

Herein we reported the synthesis of acetyl pyrazoline and cyanopyridine derivatives from 1-aryl-3-(thiophene-2yl) prop-2-en-1-ones, due to their wide range of therapeutic activities like antimicrobial, antitubercular, anti-inflammatory and antitumor. A series of acetyl pyrazolines and Cyanopyridines are obtained by reacting substituted chalcones with $NH_2NH_2.H_2O$ in glacial acetic acid and Malanonitrile with Ammonium Acetate respectively. The compounds were well-characterized by IR, NMR and Mass spectroscopic techniques and Elemental analysis.



Where R= Cl, Br, NO_2, CH_3, OH and NH_2

PP - 020

Poster Presentations

Development and validation for simultaneous estimation of rosuvastatine calcium and amlodipine besylate by liquid chromatography

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ABSTRACT

The objective of this work was to develop and validate simple, rapid and accurate RP-HPLC method for the simultaneous determination of rosuvastatin calcium and amlodipine besylate in bulk formulation. The chromatographic separation was carried out at ambient temperature on YMC Pro C_8 (150 × 4.6 mm i.d., 5 μm particle size) column using a mobile phase consisting of acetonitrile: 0.02 M phosphate buffer (45: 55 v/v, pH 3.5) at a 1 ml/min flow rate. Both the drugs were separated in less than 10 min with good resolution and minimal tailing, without any interference. The method was validated according to ICH guidelines. Quantification was achieved on PDA detector at 240 nm. The linearity of the proposed method was investigated in the range of 20-80 µg/ml (r^2 = 0.9995) for amlodipine besylate and 40-160 µg/ml (r^2 =0.9997) for rosuvastatin calcium. The limit of detection obtained were 0.03µg/ml for amlodipine besylate and 0.05µg/ml rosuvastatin calcium respectively. The limit of quantification obtained were 0.2µg/ml for amlodipine besylate and 0.3µg/ml for rosuvastatin calcium respectively. Methods was found to be simple, precise, accurate, selective and rapid and could be successfully applied for the determination of pure laboratory prepared mixtures, bulk formulations, and tablets.

PP - 021

Poster Presentations

A simple, efficient and scalable synthesis of glyoxylamide derivatives containing imidazo[1,2-a]pyridine nucleus

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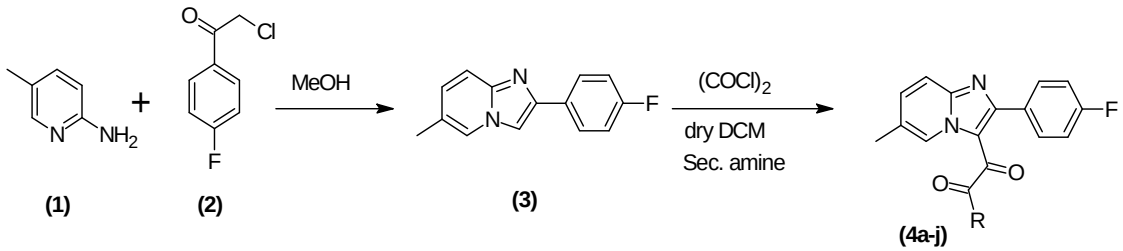
ABSTRACT

N-containing heterocycles like imidazo[1,2-a]pyridine are a class of Aza-indolizine drugs. Imidazo[1,2-a]pyridines are widely used in the field of pharmaceuticals as a anti-inflammatory, antitumor, calcium channel blocker, hypnotic, sedative, antimicrobial, antitubercular, CNS depressant, antithyroid and many other therapeutic activities. Encouraged by these result we wanted to explored the antimicrobial activity of some new imidazo[1,2-a]pyridine base glyoxylamide as this nucleus exhibit diverse pharmacology activity. We hereby reported a convenient route to synthesize imidazo[1,2-a]pyridine-3-yl-glyoxylamide derivatives and their antimicrobial activity. An improved method for the synthesis of imidazo[1,2-a]pyridine base glyoxylamide derivatives were synthesize by the reaction of 5-methylpyridin-2-amine (1) and α-haloketones (2) in methanol to give 2-(4-fluorophenyl)-6-methylimidazo[1,2-*a*]pyridine (3). Compound (3) on reaction with oxalyl chloride and different secondary amine in dry DCM to give 1-[2-(4-fluorophenyl)-6-methylimidazo[1,2-a]pyridin-3-yl]-2-(*N*,*N*-dialkylamine-4-yl)ethane-1,2-diones (4a-j). The method given in this report is quite simple, short reaction time, good to excellent yields and *in situ* reaction. The constitution of all the synthesized compounds have been characterized by using elemental analysis, FT-IR and ^{1}H NMR, ^{13}C NMR spectroscopy and further supported by mass spectroscopy. All the compounds were screened for their antimicrobial activities in progress.



PP - 022

Poster Presentations

Microwave-assisted synthesis of thiophene bearing thiazolidinone derivatives

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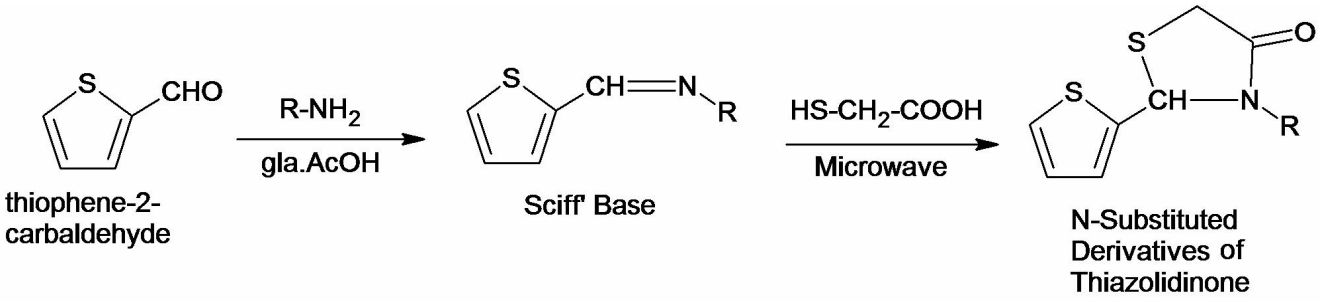
ABSTRACT

Thiazolidinones have a broad spectrum of Pharmacological properties like anti-HIV, antifungal, anti epileptic, anticonvulsant, antipsychotic etc. Extensive literature survey revealed very few published data on thesynthesis of new thiazolidinone derivatives as potential anti-HIV agents. One feasible solution is microwave-assisted synthesis, which is in many ways superior to traditional heating: reactions are completed in minutes; yields are generally higher than those achievable by traditional means. An improved method for Synthesis of thiazolidinone and it's derivatives by taken Thiophene 2-carboxaldehyde (1 mmol) and substituted amine (1 mmol) in a conical flask and 2 drops of gla.acetic acis, which produce appropriate Schiff' Base[1]. Then take Mercaptoacetic acid (2 mmol) and appropriate Schiff' base (1 mmol) in dry toluene (3 mL) were placed in a cylindrical quartz tube (Ø 2 cm). The reaction mixture was then stirred and irradiated in a microwave oven. Then neutralize the content with sat. bicarbonate solution and extract copound in ethylacetate[2]. Finally give the treatment of diethylether after removing ethylacetate, filter the seperated product and crystallize in ethanol. The constitution of all the synthesized compounds have been characterized by Elemental analyses, FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy and further supported by mass spectroscopy. The purity of the compounds have been checked by thin layer chromatography. Screening of these new heterocycles for their various anti-HIV and anti-inflammatory activities is in progress.



PP - 023

Poster Presentations

Development and validation of new quantitative gas chromatographic method for the determination of ticlopidine HCl in tablet formulation

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ABSTRACT

A new and simple gas chromatography(GC) method has been developed for determination of ticlopidine HCl in a tablet formulation. The validation of the proposed method was carried out for selectivity, linearity, accuracy, precision, recovery, limits of detection and quantification. The developed method can be used for routine quality control (QC) analysis of titled drugs in combination in tablet formulation. Ticlopidine HCl in tablets was extracted with methanol before injecting onto the gas chromatograph. The concentrations adopted were in the range of 1 to 4 mg/cm ticlopidine in methanolic solution and the accuracy obtained was 101.37±0.43 for ticlopidine HCl tablet formulation.

PP - 024

Study of stability indicating assay method development, validation and application to quality control of leflunomide by UPLC

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ABSTRACT

A simple, precise, and accurate UPLC method has been developed and validated for assay of leflunomide in tablets. Reversed-phase liquid chromatographic separation was achieved by use of ammonium acetate (0.02M)-acetonitrile 40:60(*v*/*v*) as mobile phase. The method was validated for specificity, linearity, precision, accuracy, robustness, and by stress testing of the drug(forced degradation). Response was a linear function of drug concentration in the range 10-30 μg/mL (*r*= 0.9998). Intraday and interday system and method precision were determined. Accuracy was between 99.44 and 100.24%. The method was found to be robust, and was suitable for assay of leflunomide in a tablet formulation.

PP - 025

Poster Presentations

A systematic study of stability indicating assay method for simultaneously determination of atenolol and indapamide in pharmaceutical formulation by HPLC

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ABSTRACT

A simple, precise and accurate isocratic stability indicating reversed phase HPLC assay method has been developed for the quantitative estimation of Atenolol and Indapamide in their combined dosage forms. Atenolol and Indapamide were chromatographed by using mobile phase of Acetonitrile- 0.02 M potassium dihydrogen orthophosphate (PH-3.0) buffer (50:50, v/v) at a flow rate of 0.8 ml/min and the detection was carried out at 241 nm 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 of 200-800 μg/ml and 10-40 μg/ml with a correlation coefficient 0.9995 and 0.9989 for Atenolol and Indapamide respectively. The precision (RSD) amongst six-sample preparation was 0.26% and 0.59 % for Atenolol and Indapamide respectively. For repeatability and intermediate precision (RSD) amongst six-sample preparation was 0.28 % and 0.42 % for Atenolol and Indapamide respectively. The accuracy (recovery) was between 98.83 to 99.06 % and 98.02 to 100.51 % for Atenolol and Indapamide respectively. Degradation products produced as a result of stress studies did not interfere with detection of Atenolol and Indapamide and the assay can thus be considered as stability indicating.

PP - 026

Poster Presentations

A convenient synthesis of some new glyoxylamide derivatives containing indole nucleus

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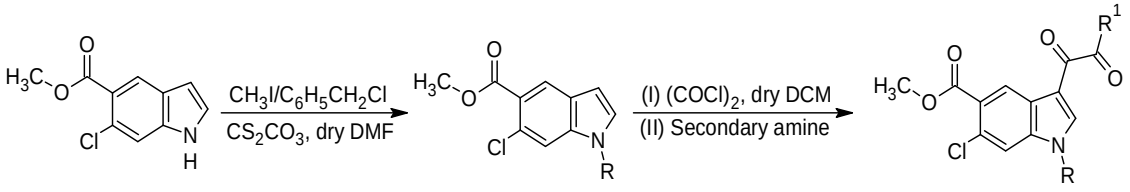
ABSTRACT

Heterocyclic compounds bearing indole ring system are potent biologically active agent has led to the exploration of large number of structural variants, containing 6-chloro-indole-5-carboxylate moiety as an invariable ingredient. Its derivative has shown various biologically activities such as anticancer, antimicrobial, anti-inflammatory, antibacterial etc. In order to develop therapeutically important compounds, it was consider of interest to synthesize some 6-chloro-indole-5-carboxylate shown as under. An improved method of some new indole base glyoxylamide derivatives were synthesized by reaction of methyl 6-chloro-1*H*-indole-5-carboxylate (1) and methyl iodide/benzyl chloride in the presence of catalyst CS_2CO_3 in dry DMF to give methyl 6-chloro-1-methyl/benzyl-1*H*-indole-5-carboxylate (2a/2b). Compounds (2a/2b) on reaction with oxalyl chloride and different secondary amine in dry DCM to give methyl 6-chloro-3-[(*N*,*N*-dialkylamino)(oxo)acetyl]-1-methyl/benzyl-1*H*-indole-5-carboxylates (3a-t). Significant enhancement in short reaction time, good to excellent yields and *in situ* reaction. The constitution of all the synthesized compounds have been characterized by using elemental analysis, FT-IR, ^{1}H NMR, ^{13}C NMR spectroscopy and further supported by mass spectroscopy. All the compounds were screened for their antimicrobial activities in progress.



(1) **(2a/2b)** **(3a-t)**

Where R = CH_3/$C_6H_5CH_2$

R^1 = Secondary amine

PP - 027

Poster Presentations

Development and validation of a stability indicating HPLC assay method for simultaneous determination of spironolactone and furosemide in tablet formulation

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ABSTRACT

The objective of current study is to developed simple, precise and accurate isocratic stability indicating reversed phase HPLC assay method and validated for determination of Spironolactone and Furosemide in solid pharmaceutical dosage forms. Isocratic RP-HPLC separation was achieved on an SGE make 150×4.6mm SS Wakosil II 5C8RS 5 µm column (Part Number : 206610 and Serial Number : A01-063) using mobile phase of Acetonitrile- Ammonium acetate buffer (50:50, v/v) at a flow rate of 1.0 ml/min and the detection was carried out at 254 nm 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 of 40-160 µg/ml with a correlation coefficient 0.9977 and 0.9953 for Spironolactone and Furosemide respectively. The precision (RSD) amongst six-sample preparation was 0.87% and 1.1 % for Spironolactone and Furosemide respectively. For repeatability and intermediate precision (RSD) amongst six-sample preparation was 0.46 % and 0.20 % for Spironolactone and Furosemide respectively. The accuracy (recovery) was between 98.09 to 100.85 % and 98.74 to 100.58 % for Spironolactone and Furosemide respectively. Degradation products produced as a result of stress studies did not interfere with detection of Spironolactone and Furosemide and the assay can thus be considered as stability indicating.

PP - 028

Poster Presentations

Synthesis of some pyridine derivatives bearing chloroquinoline analogues hetereocycles as antitubercular agents

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ABSTRACT

A survey of literature indicated that the synthesis of new hetrocyclic compounds has acquired greater importance as these compounds have a broad spectrum of antimicrobial activity. From the literature, choloroquinolines were well known for their antimalerial activity. New members of pyridine and pyrimidine have been prepared for their wide application in pharmaceutical fields.2-Amino-3- cyanopyridine derivative have been synthesized by the condensation of chalcone with malononitrile and ammonium acetate The key intermediate chalcones have been prepared by the condensation of halosubstitutedquinoine-3-carbaldehyde with different aromatic ketones in the presence of basic catalyst. All the synthesized products have been characterized using spectral technique such as IR, 1HNMR and Mass spectra. All the products have been evaluated against different strains of bacteria and fungi as well as *mycobacteriumtuberculosis*.

PP - 029

Design and synthesis of side chain modified derivatives of pyrazine by suzuki coupling reaction as anti-inflammatory and antitubercular agents

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ABSTRACT

Pyrazine and its derivatives, especially amides and sulfonamides have been used in various topics as anti-tuberculosis, oral anti diabetics, nutrition supplement, insecticides and fungicides. Extensive literature survey revealed very few published data on the synthesis of new pyrazine derivatives as potential anti-inflammatory agents. This observation prompted us to synthesize this nucleus so as to enhance the overall activities at resulting moieties can be evaluated. It was consider of interest to design and synthesize some 2-amino pyrazine derivatives shown as under. The modifications in side chain of 2-amino pyrazine have been done according to QSAR. The constitution of all the synthesized compounds have been characterized by Elemental analyses, FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy and further supported by mass spectroscopy. The purity of the compounds have been checked by thin layer chromatography. Screening of these new heterocycles for their various antitubercular and anti-inflammatory activities is in progress.

PP - 030

Poster Presentations

Synthesis and antibacterial activity of some novel fused benzenesulfonohydrazide

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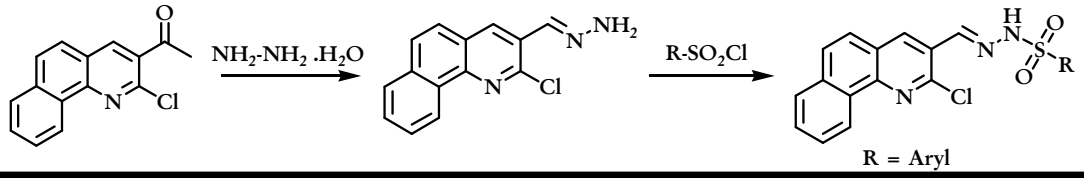
ABSTRACT

A new class of *N*'-[(2-chlorobenzo[*h*]quinolin-3-yl)methylidene]-4-methyl benzenesulfono hydrazides has been prepared from α-napthyl amine. All the synthesized compounds were characterized by IR, NMR and mass spectral data. Further, these compounds have been screened for antibacterial activities and are found to have moderate activities.



PP - 031

Ultrasonic velocity studies and allied parameters of 2- methyl benzimidazole derivatives at 298.15 K.

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ABSTRACT

The density (ρ), viscosity (η) and sound velocity (U) of solutions of 2 - methyl benzimidazole derivetives in these methanol and chloroform have been investigated at 298.15 K. Some acoustical parameters such as isentropic compressibility (K_s), Rao's molar sound function (R_m), internal pressure (π), free volume (V_f), classical absorption coefficient (α/f^2_{Cl}), viscous relaxation time (τ), apparent molar volume (ϕ_V) and apparent molar compressibility (ϕ_k) have also been determined from experimental data. A fairly good correlation between a given parameter and concentration is observed at 298.15 K. Linear or nonlinear increase or decrease of acoustical parameters with concentrations indicated existence of strong molecular interactions like solvent-solvent, solvent-solute and solute-solute interactions.

PP - 032

Poster Presentations

Novel dihydropyrimidines as a potential new class of antitubercular agents

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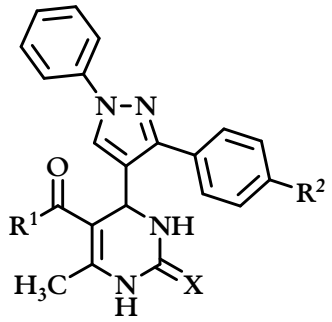
ABSTRACT

A small library of 30 dihydropyrimidines were synthesized and evaluated for their *in vitro* antitubercular activity against *Mycobacterium tuberculosis* $H_{37}Rv$. Two compounds, ethyl 4-[3-(4-fluorophenyl)-1-phenyl-1*H*-pyrazol-4-yl]-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5 carboxylate 4a and ethyl 4-[3-(4-nitrophenyl)-1-phenyl-1*H*-pyrazol-4-yl]-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate 4d were found to be the most active compounds *in vitro* with MIC of 0.02 μg/mL against MTB and were more potent than isoniazid.



4a-e to 9a-e

4a-e	X = O	$R^1 = OC_2H_5$	R^2 = 4-F, 4-Cl, 4-Br, 4-NO_2, 4-CH_3
5a-e	X = S	$R^1 = OC_2H_5$	R^2 = 4-F, 4-Cl, 4-Br, 4-NO_2, 4-CH_3
6a-e	X = NH	$R^1 = OC_2H_5$	R^2 = 4-F, 4-Cl, 4-Br, 4-NO_2, 4-CH_3
7a-e	X = S	$R^1 = OCH_3$	R^2 = 4-F, 4-Cl, 4-Br, 4-NO_2, 4-CH_3
8a-e	X = O	$R^1 = OCH_3$	R^2 = 4-F, 4-Cl, 4-Br, 4-NO_2, 4-CH_3
9a-e	X = SCH_3	$R^1 = OC_2H_5$	R^2 = 4-F, 4-Cl, 4-Br, 4-NO_2, 4-CH_3

PP - 033

Poster Presentations

Water mediated construction of trisubstituted pyrazoles/isoxazoles library using ketene dithioacetals

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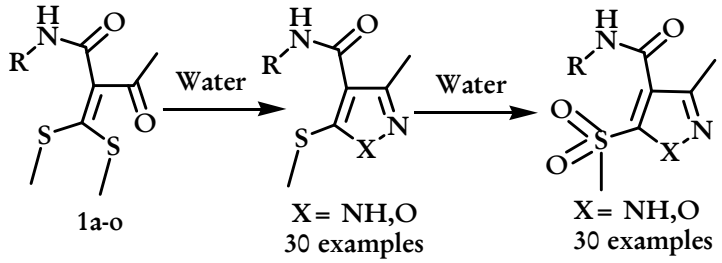
ABSTRACT

A small molecule library of alkyl, sulfone, and carboxamide functionalized pyrazoles and isoxazoles has been developed via a rapid sequential condensation of various R-acylketene dithioacetals (1a-o) with hydrazine hydrate or hydroxylamine hydrochloride, followed by oxidation of sulfide to sulfone using water as the reaction medium. An efficient and safe oxidation of sulfides (4/5a-o) to the corresponding sulfones (6/7a-o) using sodium per borate system in aqueous medium is reported. The concise and two step synthesis of trisubstituted pyrazoles and isoxazoles was investigated under variety of reaction condition. The newly developed methodology has the advantage of excellent yield and chemical purity with short reaction time using water as a solvent.



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PP - 034

Poster Presentations

Use of cyclic aliphatic ketones for spiro 2-amino-3-cyano pyrano[3,2-*c*] chromene formation

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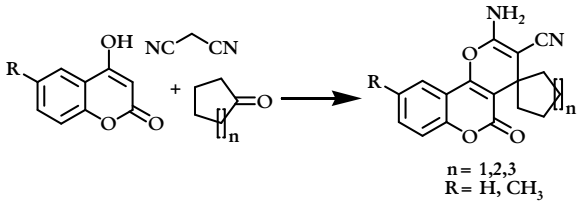
ABSTRACT

The three component reaction between 4-hydroxycoumarin, malononitrile and carbonyl compounds in ethanol in the presence of morpholine as a catalyst has been developed. Only cyclic aliphatic ketones afford spiro 2-amino-3-cyanopyrano[3,2-*c*]chromene derivatives in high yields.



PP - 035

Synthesis and antimicrobial screening of some thiazolidinone derivatives derived from diazonium salts

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ABSTRACT

Diazonium salts derived from P-Nitro aniline was coupled with salicylaldehyde in presence of strong base has afforded 5-(4-Chloro-phenylazo)-2-hydroxy-benzaldehyde.which in turn on condensation with various aromatic amines in acidic medium gave schiffs bases. It was converted into 2-[5-(4-Chloro-phenylazo)-2-hydroxy-phenyl]-3-phenyl-thiazolidin-4-one by refluxing with thioglycollic acid. These newly synthesized compounds were characterized by IR, ^{1}H NMR, ^{13}NMR, mass spectral data. All compounds were tested for antibacterial and antifungal activities. The antimicrobial activities of the compounds were assessed by the filterpaper disk diffusion plate method. The preliminary results revealed that some of the compounds exhibited promising antimicrobial activities.

PP - 036

Poster Presentations

A concise synthetic strategy to functionalized chromenones via [5+1] heteroannulation and facile C–N/C–S/C–O bond formation with various nucleophiles

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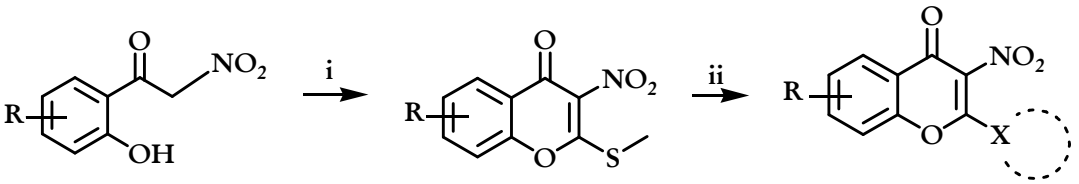
ABSTRACT

A highly efficient strategy to 2,3-substituted chromen-4*H*-ones has been developed. The methodology involves unexpected intramolecular heteroannulation of readily accessible substituted 2-hydroxy-ω-nitroacetophenone with carbon disulfide in the presence K_2CO_3 followed by methylation with methyliodide. These chromenones were further reacted with various nucleophiles such as amines, thiols, andalkoxide resulting in the facile C–N, C–S, and C–O bond formation. The scope and generality have been discussed.



i = CS_2/Base,MeI

3 examples

ii = Aryl/Alkyl amines, aryl thiiols and alkoxide

39 examples

X = N, S or O

REFERENCES

[1] Mahesh M. Savant, Neetha S. Gowda, Akshay M. Pansuriya, Chirag V. Bhuva, Naval Kapuriya, Sridhar M. Anandalwar, Shashidhara J. Prasad, Anamik Shah, Yogesh T. Naliapara.* Tetrahedron Letters 52, 2011, 254–257.

PP - 037

Poster Presentations

Construction of 3,4-dihydro-1,2-diazete ring through 4π electron cyclization of 4-hydroxy-2-oxo-2*H* chromene-3-carbaldehyde [(1*E*)-arylmethylene] hydrazone

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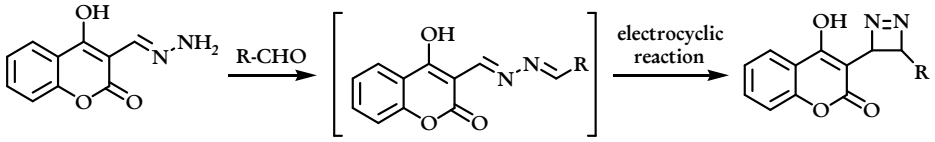
ABSTRACT

A new, short and efficient synthesis of 4-hydroxy-3-(4-aryl-3,4-dihydro-1,2-diazet-3-yl)-2*H*-chromen-2-one is described in which the 3,4-dihydro-1,2-diazete ring is constructed from arylmethylene hydrazone by 4π electron cyclization as per electrocyclic reaction.



PP - 038

Simultaneous estimation of methocarbamol and nimesulide in tablet dosage form by reversed phase high performance liquid chromatography

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ABSTRACT

An accurate and precise reversed phase high performance liquid chromatography (RP-HPLC) method has been developed for the simultaneous estimation of Methocarbamol and Nimesulide in combination in tablet dosage form. High Q Sil C-18 W column and UV detector were used and the absorption was measured at 230 nm. A mixture of Acetonitrile and Acetate buffer (pH-5) (70:30) was used as mobile phase and flow rate of 1.0 ml/min was found to be most suitable for the run time of 8 minutes. Beer-Lambert's law was obeyed in the concentration ranges 20-80μg/ml and 2-8μg/ml for Methocarbamol and Nimesulide, respectively. Limit of detection of Methocarbamol was found 0.149μg/ml and for Nimesulide it was 0.185μg/ml. The results of analysis have been validated statistically and recovery studies have been performed.

PP - 039

Poster Presentations

Etidronic acid: A new and efficient catalyst for the synthesis of novel 5-nitro-3, 4-dihydropyridimidin-2(1*H*)-ones

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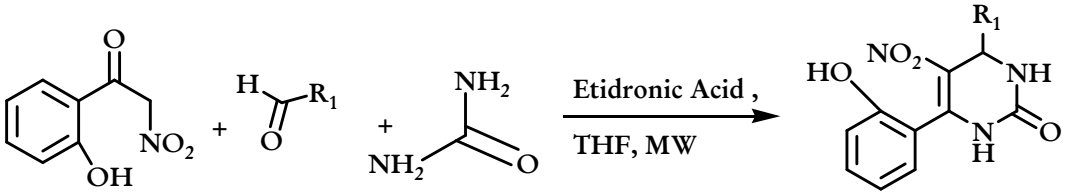
ABSTRACT

A simple, convenient and efficient one-pot cyclocondensation reaction of 1-(2-hydroxyphenyl)-2-nitroethanone, arylaldehydes and urea using etidronic acid to furnish nitro dihydropyrimidine derivatives is described. A new and efficient protocol is developed as a homogenous catalyst for dihydropyrimidines using ω– nitro acetophenone. Various bisphosphonic acids were examined to synthesized pyrimidines via multicomponent cyclocondensation reaction. This methodology has the advantage of excellent yields with short reaction time.



Where R_1 = Sub Ar-ring

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PP - 040

Poster Presentations

Microwave mediated dearylation of 2-aryloxy-5-nitropyridine

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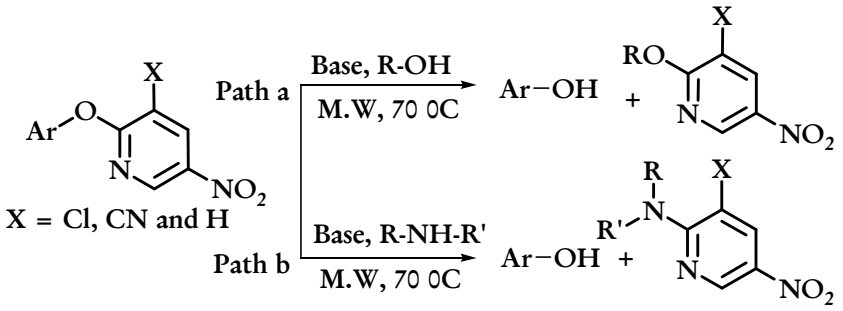
ABSTRACT

Ether cleavage reaction is widely used in organic synthesis particularly in the field of natural products and in the synthesis of polyfuctional molecules.[1-4] The cleavage of diaryl ether is involved in organic synthesis as well as in metabolic reactions.[5,6] Here we report a convenient method where 2-aryloxy-5-nitropyridine derivatives were exhibited ether cleavage reaction on treatment with alcohols/ amines in presence of base like K_2CO_3, Cs_2CO_3, NaOH, t-BuOK, etc. under microwave irradiation to yield corresponding phenols and 5-nitro-2-substituted pyridine.



Ar-OH = Quinolin-3-ol,Isoquinolin-3-ol, Naphthalen-2-ol

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PP - 041

Poster Presentations

First stereoselective total synthesis of triumfettamide

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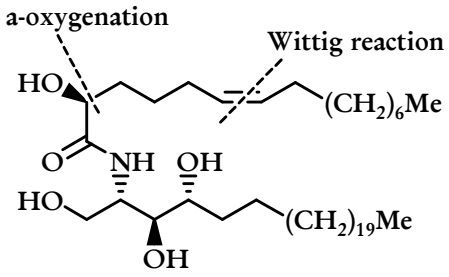
ABSTRACT

Ceramides are bioactive sphingolipid metabolites which play an important role in signal transduction and molecular recognisation processes in cell membranes. Because of its apoptosis inducing effect, studies of ceramides and its analogues become an important research area for the development of new anticancer therapeutics. Naturally occurring ceramide molecule, Triumfettamide 1, was isolated from *Triumfetta cordifolia* A.Rich, a wild shrub which is localised in the tropical Africa. It was characterised as (2S,6Z)-2-hydroxy-N-[(2S,3S,4R)]-1,3,4- trihydroxyhexacosan-6-enamide, by Ngadjui et al[1]. No synthesis of this compound has been reported till date. In the context of our ongoing programme on the synthesis of pharmacologically important natural products[2], we have developed a novel synthetic sequence of Triumfettamide 1. The details of the synthesis will be presented.



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PP - 042

Poster Presentations

First stereoselective total synthesis of debilisone 'C'

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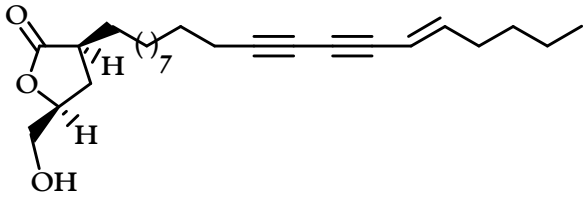
ABSTRACT

Polyacetylenes are characteristic natural products which are abundant in nature and have attracted much attention due to their biologically activity. Polyalthia debilis is a Thai herbal plant growing widely in the northeastern part of Thailand. Phytochemical investigations of the methanol extract of roots of polyalthia debilis leads to the isolation of a polyacetylene Debilisone 'C'[1]. It exhibited antimycobacterial activity against Mycobacterium tuberculosis. The minimum inhibitory concentration (MIC) of this molecule is 12.5μg/ml. Over the past few years, investigations in our laboratory have demonstrated the utility of nitroaliphatics in the synthesis of pharmacologically important natural products[2]. In this context; we have developed a practical synthesis of this molecule. The details of the synthesis will be presented.



Debilisone 'C'

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PP - 043

Poster Presentations

Synthesis of steroid-peptide conjugates using new synthetic strategies: A class of potent biologically active molecules

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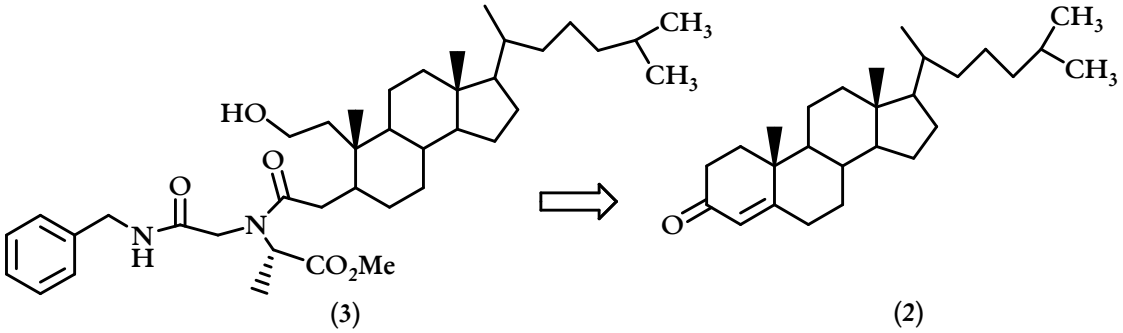
ABSTRACT

Steroid Transformation is an important area of research in chemical field. Considering the potentiality of steroid transformations, it is proposed to carry out some transformations towards the synthesis of Steroid-peptide conjugate molecules which are gaining quite importance as Peptidomimetics in recent years. It is known that conjugation of steroids to other chemically or biologically relevant molecules represents a valuable strategy to generate new properties in the resulting molecular hybrid. To the naturally occuring saponins[1], many synthetic biomolecule steroid conjugates have shown to possess many biological and physico-chemical features arising out of the junction of the two molecular entities e.g. synthetic sugar-steroid conjugates have been prepared to provide novel amphibilic molecules capable to interact with phospholipid membranes. Similarly peptide-steroid conjugates have been used as synthetic receptors of oligopeptide sequences, as protease-like artificial enzymes and as mimics of the natural cationic peptide antibiotics. Indeed this objective requires the production of novel reagents and improved methodologies towards the improvement in the conjugation process[2].



(3) (2)

Scheme 1 : Represents the synthesis of steroid-peptide conjugate 3 Starting from 3-oxosteroid derivative 2.

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PP - 044

Poster Presentations

The effect of hydroalcoholic extract of *chlorophytum borivilianum* Sant. F. on sexual motivation and behavior in the female rats

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ABSTRACT

The present investigation examined the effect of hydroalcoholic extract of *Chlorophytum borivilianum* Sant. F. (CB) on the sexual motivation and copulatory behavior of female rats. In first experiment, 36 sexually experienced female rats were tested in a runway for their motivation to approach empty goalbox, a non estrous female and adult male. The evaluation parameters were run time, proximity time and retreats. Subjects were tested in both nonestrous and estrous state, and following administration of 100, 300 and 500 mg/kg of CB for 21 days. Results indicated that the pretreatment with ovarian hormones significantly increased the sexual motivation of the subjects. Furthermore, CB treatment significantly improved the sexual motivation after 11 and 21 days of treatment period. In second experiment, 24 female subjects (estrous phase) were individually paired with an adult sexually experienced male rat for 30 minutes copulatory test, on 11th and 21st day after pretreatment with either vehicle (2 ml/rat/day) or CB (100, 300 and 500 mg/kg). Results indicated the significant increment in emission of proceptive behaviors like hops, darts, ear wiggling and solicitations, suggestive of increased sexuality in the females treated with CB. Various rejection responses of females towards their male counterparts were significantly reduced after pretreatment with various doses of CB. Lordosis quotient, as a measure of receptive behavior was unaffected by pretreatment with CB. To conclude, CB treatment significantly increased sexual motivation and behaviors of female rats, suggesting its probable role and possible use in the treatment of females with reduced libido and sexuality.

PP - 045

Poster Presentations

Ethnomedicine: An unexplored path of drug discovery

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ABSTRACT

Ethnomedicine is the study of traditional medical practice centered around cultural interpretation of health and disease. It has been the source of healing since centuries. It is multi-disciplinary and involves use of plants, spirituality, environment and incorporates conventional biology, ethnobotany and ethnopharmacology[1]. Ethnobotany Genomics involves biotechnology and biodiversity, thereby aiding identification of particular plant species used for particular disease[2]. Spirituality is an integral component of ethnomedicine and despite lack of scientific validation, institutions in USA are incorporating it into their services[3]. Ethnomedicine has been ignored by health practitioners due to uncertainty of chemical constituents, dosage and toxicity of plants[4]. However, it is the most successful path used by the pharmaceutical industry in finding novel therapeutic constituents[5]. According to WHO, ethnomedicine has maintained its popularity in developing countries and its use is increasing exponentially in industrialized countries. 80% of world population relies on plants for healthcare. In India, 70% population prefers Ayurveda, which is the oldest system of medicine. In China, almost all people rely on Chinese traditional system of medicine. Out of top 150 drugs in USA, 57% contain active compound derived from plants. Annual global market for herbal medicines is currently over US $60bn[6]. This makes exploration of ethnomedicinal practices the need of the hour. Pharmacognostical, phytochemical and clinical evaluation of ethnomedicinal claims will benefit the healthcare system because of its affordability and sustainibility. Indian industries can lead the pharmaceutical sector if Ayurveda and IPR are tapped efficiently.

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PP - 046

Poster Presentations

Synthesis of substituted 6h-dibenzo [b, d] pyran and pyranone derivatives as potential selective estrogen receptor modulators

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ABSTRACT

Recently, the dibenzopyranone/pyrans and naphthopyran nucleus have surfaced as common ring system of a group of antibiotics, antibacterials, antitumors and immunomodulators, etc. exemplified by alternariol, ravidomycin, shilajit, ellagic acid etc. and have also been reported to posses antidepressant, 5α-reductase, aldose reductase, 3-phospho glycerate kinase inhibitors activities. A series of 3,4-carbocyclic/ heterocyclic fused ring systems incorporating dibenzo [b,d]-pyran pharmacophore have been reported as a novel class of non-steroidal estrogen antagonist and progesterone agonists. Several 3:4-carbocyclic and heterocyclic compounds have recently been reported in literature such as KCA-098, LY-356156, and coumestrol analogue etc. which selectively modulate the activity of estrogen receptor (ER). Our continuing effort on the development of 2,3-diarylbenzopyrans as selective estrogen receptor modulators led us to synthesize some dibenzopyranone/pyran molecules as potential antiestrogenic agents. As a critical balance of estrogenic as well as antiestrogenic effect is required in a molecule, therefore, various structural modifications at C-3, 6, 8 and 9 positions were done in the molecule to study structure-activity relationship and evolve a novel selective estrogen receptor modulator.

PP - 047

Determination of atmospheric concentration of poly aromatic hydrocarbons by high performance liquid chromatography

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ABSTRACT

Polycyclic aromatic hydrocarbons (PAHs) are group of chemicals formed during the incomplete combustion of wood and fuel. Exhaust from diesel, engines contains lower concentrations of some gaseous pollutants but higher concentration of particulate, bearing organic extract PAHs. Air borne particulate matter from the atmosphere of the city of Lucknow was collected on the filter paper which is made up of cellulose nitrate with quartz fibers. Poly aromatic hydrocarbons (PAHs) and associated with air borne particulate matter were extracted by Soxhlet procedure and analyzed by HPLC. The concentration of all the four zones were determined.

PP - 048

Poster Presentations

Synthesis of B-ring annelated steroidal pyrazoles under microwave irradiation

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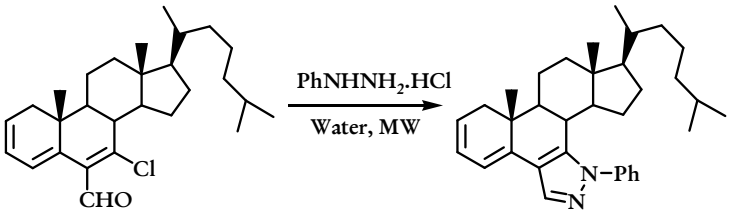
ABSTRACT

Pyrazole moiety constitutes the key sub-unit of many pharmacologically important compounds having wide range of biological activities such as antipyretic, analgesic, anti-inflammatory, hypoglycaemic and sedative-hypotonic activities[1]. The pyrazole unit is the core structure of a number of natural products[2] and is the building block of fused heterocycles like pyrazoloisoquinolines[3], pyrazolopyrimidines[4] and pyrazolopyrazines[5], which are widely used in pharmaceutical industries. Steroidal pyrazoles, in which, a pyrazole nucleus is fused to a steroid moiety, also constitute a class of medicinally important compounds. Boruah et.al[6] has already developed a novel strategy for the synthesis of A- and D-ring annelated steroidal pyrazoles from the corresponding β-formylenamides. Owing to the biological activities of steroidal pyrazoles, we aim to synthesize some B-ring annelated steroidal pyrazoles by treatment of 7-chloro-6-formyl steroids with phenyl hydrazine in aqueous medium under microwave irradiation.



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PP - 049

Poster Presentations

Total synthesis of xanthohumol and some of its analogues

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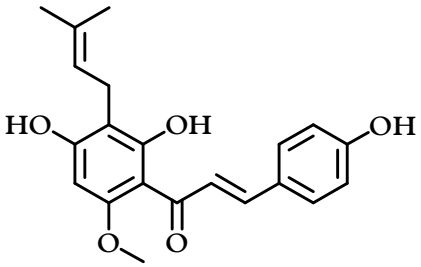
ABSTRACT

Nature is a source of potential therapeutic agents and lead compounds that have provided the basis and inspiration for the semisynthesis or total synthesis of effective new drugs. Xanthohumol is a prenylated chalcone present in the hop plant *Humulus lupulus* which is added to beer to impart bitterness and ?avor[1]. Xanthohumol has been found to have a range of interesting biological properties *in vitro* that may have therapeutic utilities for the relief of hot flashes, for treating osteoporosis, atherosclerosis and inhibition of HIV-1 as well as a potential broad-spectrum anticancer and cancer prevention agent[2]. Studies directed toward dietary supplements having Xanthohumol content are increased and there are reports of its introduction to the market to address a wide range of health issues, including fighting oxidative stress, regulating fat metabolism, helping maintain healthy glucose and cholesterol levels, eliminating toxins, modulating hormone levels and supporting eye health[3]. Here we want to report a simple route for the total synthesis of Xanthohumol as well as some of its analogues from acetophenone derivatives.



Xanthohumol

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PP - 050

Poster Presentations

Selective oxidation of hydrazides using *o*-iodoxybenzoic acid to carboxylic acids, esters, and aldehydes

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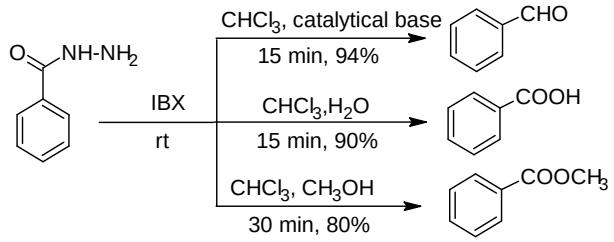
ABSTRACT

A selective method for conversion of hydrazide to corresponding aldehydes, acids, and esters by using hypervalent iodine reagent o-iodoxybenzoic acid (IBX) has been developed under different reaction conditions. (Takale et al.[1]) The method is mild and gives good yields for both aliphatic and aromatic substrates. Hydrazides are important intermediates required in protection and deprotection of carboxylic acids. However, potential utility and applicability as a protecting group are diminished considerably owing to high hydrolytic stability. Hence, much less work has been done for deprotection of hydrazide and thus deprotection of hydrazide to the corresponding acid using mild conditions is of great interest. Previous reported methods used benzeneseleninic acid anhydride, (Back et al.[2]) etc. however; all these methods require either toxic metals or tedious work up procedure. Hypervalent iodine reagents have found widespread applications in organic synthesis because of their selectivity and simplicity in use. Our group has been working extensively on the development of novel methodologies under mild reaction conditions using various hypervalent iodine reagents like IBX. (Telvekar et al.[3])



Scheme:- Conversion of benzhydrazide into benzaldehyde, benzoic acid and methyl benzoate using IBX at room temperature

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PP - 051

Poster Presentations

Pthalimide derivatives as possible spermicides with dual protection

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ABSTRACT

The acquired immune deficiency syndrome (AIDS) appears to thrive in the presence of over-population, poverty and other sexually transmitted diseases (STDs).The existed marketed molecules for spermicidal activity have lots of risk to prevent such conditions. Therefore, developing user controlled non-detergent, topical vaginal spermicides that can provide protection against pregnancy as well as common sexually transmitted pathogens has become an urgent global priority. As per literature review, cyclic imides, such as succinimide, maleimide and phthalimide possess structural features, which confer potential biological activity and pharmaceutical use. Taking the above information in view, the derivatives of pthalimide were synthesized and evaluated for their spermicidal as well as antifungal and antibacterial against candida, aspergillus and gram +ve and gram-ve spp. Nonoxynol-9 was used as reference standard for biological evaluations. All the synthesized compounds were identified by ^{1}H-NMR, mass spectra and elemental analysis. The study demonstrated that the incorporation of carbodithioic acid residue in pthalimide leads to a potent spermicidal activity along with moderate antifungal and anti bacterial activity. In conclusion, synthetic derivatives showed similar spermicidal profile along with moderate antifungal and anti bacterial activity as compare with nonoxynol-9. It could be a viable alternative for nonoxynol-9 which has the tendency to increase the risk of HIV transmission.

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PP - 052

Poster Presentations

2-(2-hydroxy-3-methoxybenzlideneamino)-2-methylpropane-1, 3-diol and phenanthroline based metallodrugs (Co(II), Cu(II) and Zn(II): Their *in vitro* DNA binding and cleavage studies, SOD and antitumor activity

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ABSTRACT

To illustrate the chemotherapeutic preference of phen containing SOD metallodrugs targeting DNA, Co(II), Cu(II) and Zn(II) complexes 1 - 3 ,respectively have been isolated and thoroughly characterized by various (IR, ^{1}H,^{13}C NMR, EPR, Magnetic Susceptibility, ESI-MS, UV-vis) spectroscopic and analytical methods. The SOD activity of the complexes 1-3 was determined by using nitro blue tetrazolium (NBT) assay. The interaction studies of 1 -3 with CT-DNA was followed by electronic absorption and luminescence titrations which reveal greater DNA binding propensity of 1 as compared to 2 & 3. Further confirmation of DNA binding was achieved by studying nuclease activity of 1 - 3 with supercoiled pBR322 DNA. Interestingly, the cleavage mechanism exhibited by 2 is likely to involve oxidative pathway. On the contrary, 1 and 3 followed hydrolytic pathway, albeit in alteration of superhelicity of plasmid DNA by 1 is an additional unique feature facilitating the formation of complex 1-DNA adduct. While complex 1 &3 possess SOD activity with IC_{50} values 0.73μM and 11.29μM respectively, the best activity was revealed by Cu(II) complex 2 with IC_{50} value as 0.53μM. Complex 2 and 3 successfully exhibited antitumor activity over a broad range of varying cell lines which was determined by SRB assay, while 1 is still under investigation. These results imply a key role of varying metals, in designing novel SOD based anticancer agents.

PP - 053

Poster Presentations

In vitro DNA binding studies and cleavage activity of new chiral copper-aminoacid ternary complexes

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ABSTRACT

A robust cancer chemotherapeutic agent should meet the prerequisite criteria of drug design which includes (i) good DNA binding ability (ii) specific tagging to drug target at molecular level (iii) preferential selectivity to DNA base sites / minor groove or major groove binding (iv) reduced toxicity and better cellular uptake. In the light of above, we have designed and synthesized new L and D copper-amino acid ternary complexes 1-3 (a and b), bearing bioactive benzimidazole pharmacophore ligand scaffold. These complexes were thoroughly characterized by analytical and spectroscopic studies viz., IR, EPR, mass spectroscopy. In vitro DNA binding studies and cleavage activity of these complexes was carried out to ascertain their potential to act as antitumor agents. DNA-binding studies reveal that both the enantiomers bind to CT DNA via electrostatic interaction involving phosphate backbone of DNA, in addition to the coordinate covalent interaction to N7 of guanine base of DNA helix. However, the L- enantiomeric form show better DNA binding propensity to CT DNA, these complexes bind more avidly and strongly as was ascertained by their intrinsic binding constant (K_b) values which were of the order 1a > 2a > 2b > 3a > 3b > 1b. Cleavage activity is often closely related to DNA binding ability and to the therapeutic potential of the drug candidate. Therefore, cleavage studies of complexes 1 (a and b) (employing agarose gel electrophoresis) with pBR322 DNA was carried out and concentration dependent cleavage experiments reveal that both complexes cleave DNA efficiently involving oxidative cleavage mechanism. Further investigations regarding the mechanistic pathway are still underway.

PP - 054

Poster Presentations

Design and synthesis of chiral CuII / SnIV bimetallic metal based potential antitumor agent: Preliminary *in vitro* DNA binding and cleavage activity

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ABSTRACT

New heterobimetallic complexes possessing (CuII/SnIV and NiII/SnIV) bimetallic cores were synthesized from their monometallic Cu(II) 1 and Ni(II) 2 complexes by de novo design strategy involving a chiral biologically active ligand scaffold. All the complexes were thoroughly characterized and the proposed structure of the complexes was formulated on the basis of elemental analysis and other spectroscopic data including 1H, 13C and 119Sn NMR in case of 2 and 4. Ni–Sn heterobimetallic analogue 4 was synthesized for NMR structure elucidation. Preliminary in vitro DNA binding studies viz. UV-visible, fluorescence, cyclic voltammetry and viscosity measurements were carried out. These complexes exhibit significant hyperchromicity on addition of DNA indicative of electrostatic mode of binding. Cu-Sn heterobimetallic complex has novelty due to molecular scaffold which ensures a dual mode of binding and preferential selectivity inside the cells (Cu(II) ions specifically bind to N7 guanine residue of DNA while Sn(IV) ions prefer to bind the phosphate backbone of DNA helix). Furthermore, the Cu-Sn heterobimetallic complex 3 exhibited avid DNA binding propensity as quantified by Kb, Ksv values and shifts in the peak potential values. DNA binding propensity of 3 was also validated by its artificial nuclease activity with supercoiled pBR322 DNA; complex 3 exhibits a remarkable DNA cleavage activity (concentration dependent) with pBR322 DNA and the cleavage activity of 3 was significantly enhanced in presence of activators and activating efficiency follows the order H2O2 > Asc > MPA > GSH, and further it was observed that cleavage reaction involves various singlet oxygen species and hydroxyl radicals via hydrolytic cleavage mechanism. The complex 3 is accessible to major groove.

PP - 055

Poster Presentations

A novel application of (diacetoxyiodo)benzene for carbon-carbon Cleavage of aryl diamines and synthesis of quinines

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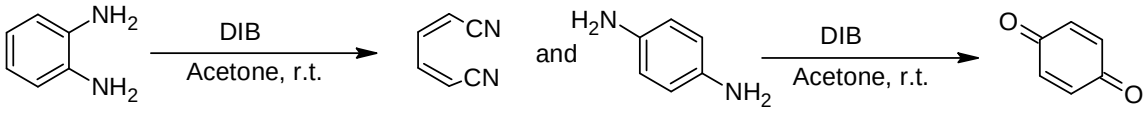
ABSTRACT

A first novel synthetic utility of hypervalent iodine reagent, (Diacetoxyiodo) benzene (DIB) for diamino aryl carbon-carbon cleavage is described. 1,2 diamino aryl compounds successfully converted into corresponding nitriles, while the developed method also useful for the preparation of quinone from corresponding 1,4 diamino aryl compounds.[Telvekar et al.(1)] The advantages of this protocol are shorter reaction time and mild reaction conditions to obtain moderate to good yields. DIB is a hypervalent iodine reagent which is readily available and frequently used in several oxidative transformation. [Kotali et al.(2)] During the course of our studies, we found that treatment of DIB to 1,2-diaminobenzene in acetone resulted into formation of *cis, cis*-mucononitrile by oxidative cleavage of carbon-carbon bond. It was interesting to know that under these reaction conditions 1,3-diaminobenzene was unaffected while 1,4-diaminobenzene showed unexpected results by formation of benzoquinone rather than expected fumaronitrile and provided an interesting route to quinines. The relevant of this methodology stems from the fact that all the aforementioned transformations are quite fundamental in nature and can be easily applied to a multitude of synthetic strategies. Investigations from our laboratories have revealed a series of new paradigm for hypervalent iodine mediated reactions under mild conditions.[Telvekar et al.(3)]In conclusion, we exploited a novel application of DIB for oxidative cleavage of carbon-carbon aryl diamines, to nitriles as well as a novel route for synthesis of quinones is describe in short reaction time. Both these applications are general, practical, economical, and efficient.



Scheme 1: Oxidative conversion of aryl diamines using DIB and acetone as a solvent at R.T.

PP - 056

Poster Presentations

The discovery of 3-((5-phenyl-1,3,4-oxadiazol-2-yl)thio)benzo-[b]thiophene 1,1-dioxide based inhibitors of tumor necrosis factor-alpha (TNF-α) production

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ABSTRACT

Tumor necrosis factor-α (TNF-α) plays an important role in the pathology of various auto-immune/inflammatory diseases including rheumatoid arthritis (RA), psoriasis and inflammatory bowel disease. In clinical trials, Remicade (the monoclonal TNF-α antibody; infliximab), and Enbrel (the soluble TNF p75 receptor fusion protein; TNFRp75:Fc; etanercept), have been shown to be effective in the treatment of RA and Crohn's disease. In spite of the widespread use of these biologics, up to 50% of patients treated with TNF blockers fail to improve disease status significantly. Furthermore, the use of these biologic agents is associated with certain limitations (e.g., parenteral route of administration, high cost of therapy, risk of opportunistic infections, induction of allergic reactions, activation of latent tuberculosis, increased risk of cancer, risk for worsening congestive heart disease). Hence, there is an unmet medical need for orally active inhibitors of TNF-α that would have the same effect as biological agents but without the undesirable side effects. Our quest for such therapeutics prompted us to investigate small molecules which will inhibit the production of TNF-α. We screened in-house library compounds for TNF-α inhibitory activity in the lipopolysaccharide (LPS)-stimulated human peripheral blood mononuclear cells (hPBMC) assay. Several compounds inhibited TNF-α production in the hPBMC assay with an IC_{50} in the range of 0.15–1.2 μM. Based on these initial findings, 3-((5-phenyl-1,3,4-oxadiazol-2-yl)thio)benzo[b]thiophene 1,1-dioxide scaffold was chosen to further improve upon the TNF-α inhibitory activity. Structural alterations led to 2 compounds from this series demonstrating moderate inhibitory activity in the *in vivo* LPS-induced TNF-α production assay in BALB/c mice. The moderate *in vivo* TNF-α inhibitory activity of these compounds can be attributed, at least in part, to their poor plasma stability and inferior PK profile. Chemical modifications aimed towards overcoming these liabilities will be discussed.

PP - 057

Poster Presentations

A simple and efficient one-pot synthesis of 4-thiazolidinones in poly(propylene glycol)

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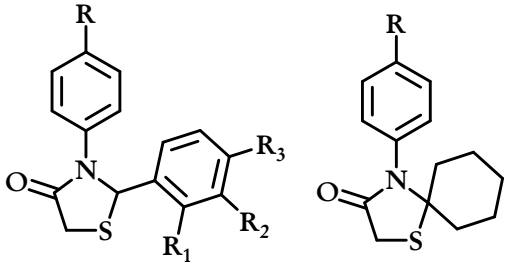
ABSTRACT

4-Thiazolidinones are an important class of biologically active five membered heterocycles. These molecules have received significant attention during the last decade due to their diverse pharmacological profiles as anticonvulsant, anti-HIV, antifungal, antibacterial and COX-1 inhibitors[1]. Various methods[2-5] are available in the literature to synthesize 4-thiazolidinones via a condensation cyclization reaction of an amine with a ketone or an aldehyde and thioglycolic acid but the design of simple, economical and efficient synthetic strategy for the construction of these molecules is highly desired. In view of enormous pharmacological potential of this class of compounds, we have successfully devised a simple, economical and robust one-pot three-component synthesis of these heterocycles in good to excellent yields (60-97 %) using polypropylene glycol (PPG) as a solvent medium. Details of this synthetic protocol will be discussed in the poster.



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PP - 058

Poster Presentations

Cyclohexane-1,2-diamine derivatives: Synthesis and antimicrobial activity evaluation

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ABSTRACT

The discovery of antimicrobials like penicillin and tetracycline paved the way for better health for millions around the world. However, with the development of antimicrobials, microorganisms have developed resistance against widely used antimicrobials hence there is an urgent need to develop new antimicrobial agents, that can solve the problem of drug resistance. Chemotherapeutic principles of various amine derivatives have been known either as therapeutic agents or as biological tools since the beginning of medical history.[1] Antimicrobial and antiparasitic activities of amines and polyamines based on spermine and spermidine is already known and interestingly their antitubercular activity is enhanced by increase in hydrophobic character. Despite the availability of curative chemotherapy and a vaccine tuberculosis (TB) continues to be a major public health threat.[2] The World Health Organization (WHO) estimates that 9.27 million new cases of TB occurred in 2007.[3] 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. *N*-Alkyl benzylamines *viz.* bromohexine and ambroxol isolated from Indian shrub *Adhatoda vasicca* are widely used as mucolytics have shown pH-dependent growth inhibitory effect on *Mycobacterium tuberculosis*.[4] As a part of our ongoing efforts towards the synthesis of novel antimicrobial agents, we became interested to modify the bromhexine molecule.[5,6] A number of symmetrical and unsymmetrical cyclohexane-1,2-diamine hydrochloride salts were synthesized and evaluated for their antibacterial as well as antitubercular efficacy.[7] These compounds were found to have potent activity against *M. Tuberculosis* $H_{37}Rv$ and the four bacterial strains *viz. E. coli*, *P. aeruginosa*, *S. aureus* and *S. epidermidis* without any hemolytic activity at very high concentration.[8]

PP - 059

Poster Presentations

Synthesis and antimalarial activity evaluation of tetraoxane based compounds

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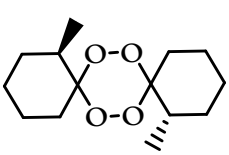
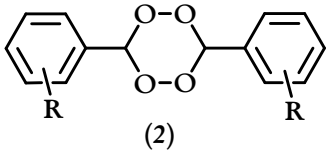
ABSTRACT

Endoperoxides have attracted attention of chemist and biologist since last two decades due to their potent activity against malarial parasite[1]. Artimisinin and its semisynthetic derivatives represent the endoperoxide class of compounds, which exhibits antimalarial activity against chloroquine-resistant strain of *Plasmodium falciparum*. Extensive mechanistic studies revealed that peroxide linkage is essential for the antimalarial activity of these compounds[2,3]. In recent years antoher class of compound namely dispiro-tetraoxanes received much attention due to its artemisinin like activity[4]. However, structural diversity of this important class of compounds is not available[5]. As a part of our ongoing programme towards the development of novel antimalarial[6-8] we synthesized symmetrical and asymmetrical tetraoxanes using substituted benzaldehydes as starting materials. In order to improve the bioavaibility of these compounds efforts were made to hook-up these compounds to another antimalarial pharmacophore or to a basic moiety. To this end, synthesis and antimalarial activity evaluation of tetraoxanes and tetraoxane based hybride compounds will be presented[9-12].

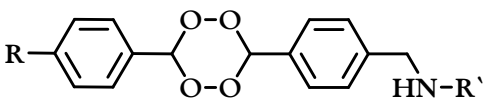


(1)

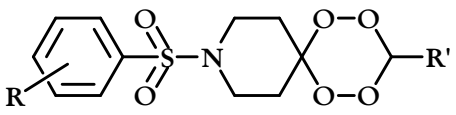


(2)

(MIC = 0.35 - 13.9 (μM))

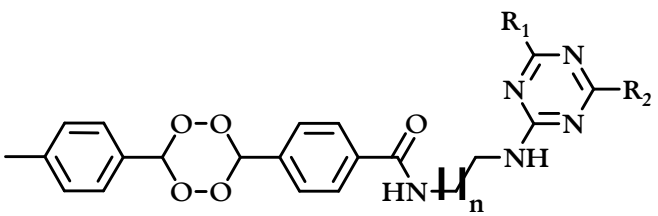


(3)



(4)

R = CH_3
= H



(5)

R_1 and R_2 = different aromatic and aliphatic amino groups

PP - 060

Poster Presentations

4-aminoquinoline based hybrid molecules: Synthesis and antimalarial activity evaluation

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ABSTRACT

Malaria poses a great threat to public health and about 50% of world population is at risk of suffering from malaria[1]. Among the four *Plasmodium* species that cause malaria, *P. falciparum* is the most dangerous and causes severe malaria[2]. The worldwide increase in drug-resistance to many of the existing antimalarials such as chloroquine and others, has brought a serious emergence in the search and development of new antimalarial agents active against drug-resistant *Plasmodium* strains. 4-Aminoquinoline class of therapeutics, to which chloroquine belongs, are the most widely studied antimalarials as they are easy to prepare, have good pharmacokinetic property and show low toxicity and side effects[3]. It has been found that modification of the basic side chain of chloroquine by linking it with other antimalarial entities such as triazines and pyrimidines can lead to improved 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), 4-aminoquinoline-triazole (2 and 3) and 4-aminoquinoline-pyrimidine (4) 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 - 061

Poster Presentations

Synthesis of pyrazino [2,1-*b*] quinazolines via a microwave-assisted transition-metal-catalyzed regioselective cyclization

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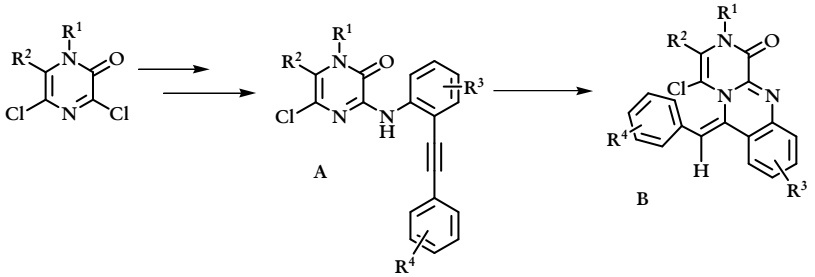
ABSTRACT

The transition-metal-catalyzed intramolecular cyclization between alkynes and nitrogen is one of the most important routes for the synthesis of nitrogen containing heterocycles.[1] As part of our continuous interest in the chemistry of 2(1*H*)-pyrazinones[2], an efficient transition-metal-catalyzed process for the generation of tricyclic N-fused heterocycles has been developed. This transformation proceeds via a microwave-assisted[3] silver-catalyzed[4] 6-exo-dig cyclization of intermediate A, leading to the formation of pyrazino[2,1-*b*]quinazolines in good to excellent yields. A detailed overview will be given describing our recently developed and optimized protocol.



PP - 062

Poster Presentations

An expeditious route towards pyrazine containing nucleoside analogue

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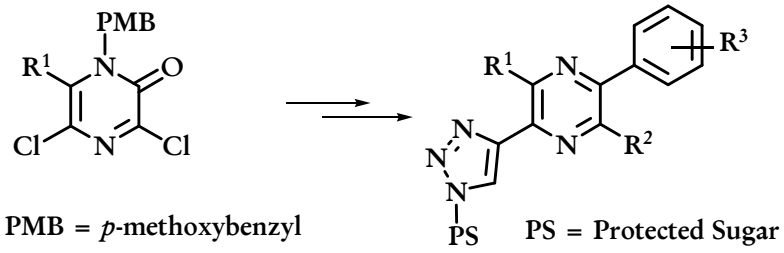
ABSTRACT

A new strategy for the synthesis of asymmetrically tri- and tetra-substituted pyrazines[1] starting from *para*-methoxybenzyl-protected 3,5-dichloro-2(1*H*)-pyrazinones, has been elaborated. The migration of the para-methoxybenzyl group and a Liebeskind-Srogl[2] cross-coupling reaction on S-PMB are the key steps.



PMB = *p*-methoxybenzyl PS = Protected Sugar

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PP - 063

Poster Presentations

Forced degradation study on amisulpride and application of validated stability-indicating isocratic liquid chromatographic method in stability testing of amisulpride tablets

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ABSTRACT

Forced degradation on Amisulpride was studied under the conditions like hydrolysis, oxidation, dry heat and photolysis and an isocratic stability-indicating HPLC-UV method was developed and validated. The separation was carried out by using a reversed-phase C18 column (250 × 4.6 mm, 5μm). The retention time of Amisulpride and its impurity (Imp-B) are 28.49 min and 32.45 min respectively with sharp peak shapes and resolution greater than 3.0. Results of the analysis were validated statistically and by recovery studies. The proposed method can be successfully used to determine the drug contents of marketed formulations and in stability testing of Amisulpride tablets.

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PP - 064

Poster Presentations

Synthesis, characterization and biological activities of transition metal complexes derived from Schiff base of o-phenylenediamine and P-dimethylaminobenzaldehyde

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ABSTRACT

The transition metal complexes of *N*-{(*Z*)-[4-(dimethylamino)phenyl]methylidene} benzene-1,2-diamine (1.C) of o-phenylenediamine (1.A) and P-dimethylaminobenzaldehyde (1.B) have been prepared and characterized by physical measurements like elemental analysis, spectroscopic methods (^{1}H NMR, C^{13} NMR, IR and UV-VIS Reflectance), thermal and magnetic studies. The metal complexes have been synthesized by simple metathetic reaction between transition metal salts of $CrCl_3$, $Fecl_3$, $CoCl_3$, $NiCl_2$, $CuCl_2$ and Schiff base in 1:1 molar ratio (in hot distilled water- ethanol 1:1 mixture). The Schiff base and metal complexes have screened for their antibacterial and antifungal activity.

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PP - 065

Poster Presentations

Oxidative decarboxylation of aryl carboxylic acid using (diacetoxyiodo) benzene for preparation of aryl aldehydes, ketones, and nitriles

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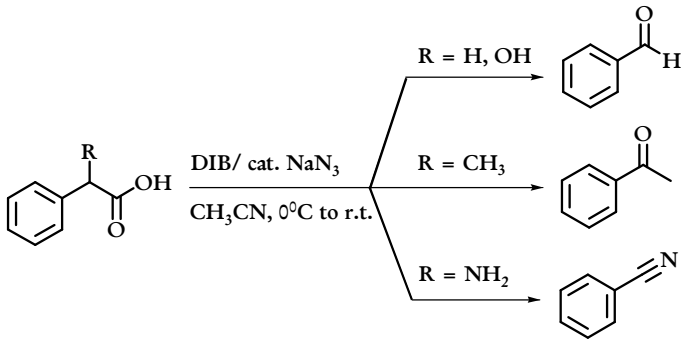
ABSTRACT

A novel synthetic application of hypervalent iodine reagent (diacetoxyiodo)benzene, and catalytic amount sodium azide in acetonitrile for decarboxylation of 2-aryl carboxylic acid into corresponding aldehydes, ketones and nitriles at room temperature is done[1]. The advantage of this protocol is shorter reaction time and mild reaction condition to obtain good yield. Hypervalent iodine reagent have attracted increasing interest and use in various oxidative transformation because of their selective, mild nature[2]. We observed that (diactoxyiodo)benzene reagent could be used with catalytic amount of sodium azide for oxidative transformation of aryl carboxylic acid to corresponding aldehydes, ketones and nitriles. Oxidative decarboxylation of mendalic acid to aldehyde or ketone can be done with various oxidizing reagent such as chromic acid, sodium bismuthate[3], whereas oxidative decarboxylation of α-amino acid can be converted in to their nitriles done with the help of N-bromo succinimides, alkaline bromide[4]. For our initial studies we have chosen phenyl acetic acid as model substrate which stirred with (diacetoxyiodo) benzene and catalytic sodium azide in acetonitrile at room temperature. It was interesting to know that without sodium azide reaction does not take place. During the further study it was found that 2-phenyl propanoic acid, mendalic acid and alpha-amino acetic acid can be successfully converted into corresponding, benzaldehyde, and benzonitrile. In summary we have presented novel application of (diacetoxyiodo) benzene for oxidative decarboxylaition of 2-arylcarboxylic acid to aldehydes, ketones and nitrile at room temperature.



Scheme 1: Oxidative decarboxylation of phenyl acetic acid into corresponding benzaldehyde, ketone and benzonitrile

PP - 066

Poster Presentations

Synthesis and antimicrobial screening of substituted-5-imidazolones

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ABSTRACT

Imidazole nucleus constitutes a special moiety found in several therapeutic agents and this heterocyclic system provides an interesting theme for the synthesis of various biologically active compounds. A number of naturally occurred imidazoles are found to have very interesting pharmacological activity. As a part of our investigation for developing efficient method for the synthesis of 1-substituted-4-arylidene-2-substituted styryl-2-imidazolin-5-one, different N-substituted amino acids and 2- substituted aminocinnamanilides was cyclised in presence of an aromatic aldehydes and amines. All these synthesized compounds have been characterized by spectroscopic method and submitted for evaluation of their biological activities. Some of these compounds shows very good fluorescent properties and work is in progress.Construction of somewhat complex organic molecule generally involves several steps , in the present method all the steps are telescoped and synthesis was accomplished in one flask and the present one flask synthesis is simple and quick and the work up is easy.

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PP - 067

Poster Presentations

AV2010-39: A new broad spectrum antifungal from streptomycetes sp.

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Piramal Life Sciences Limited

ABSTRACT

Fungal infections range from superficial conditions of the skin and nails to disseminated life-threatening diseases. Serious invasive fungal infections caused by Candida spp., *Cryptococcus neoformans*, Aspergillus spp., *Pneumocystis carinii* and *Histoplasma capsulatum*, represent an increasing threat to human health. The present antifungal agents show some limitations, such as the significant nephrotoxicity, emerging resistance, narrow spectrum of action. Hence the development of new antifungal agents is an urgent medical need. In course of our search for new antifungal compounds we isolated the new antifungal compound AV2010-39 by bioactivity guided isolation from an actinomycetes and by various chromatographic and spectroscopic studies. The actinomycetes strain NPAc10240 was isolated from a soil sample composed from Himachal Pradesh. The strain was characterized according to classical microbiological methods and by 16S rRNA method. The strain has closest match with *Streptomyces rectiviolaceus* (98%) and *Streptomyces viridocyaneus* (98%). During isolation of the compound the antifungal bioactivity was monitored by agar well diffusion assay using fungal test models such as Aspergillus *fumigatus*, *C. albicans* (I.V.), *C. albicans* ATCC 14503, *C. krusei* GO6, *C. krusei* GO3, *C. glabrata* HO4, *C. glabrata* HO5, *A. fumigatus* ATCC 16424, *Cryptococcus neoformans, Trichophyton* sp. The MIC of AV2010-39 was evaluated by Broth macro dilution method according to NCCLS guidelines as per document no. M27-A3, NCCLS, Wayne fungi and yeasts. The mean MIC for *C. albicans* and *A. fumigatus* was between 8-16μg/ml and for the fluconazole resistant *C. albicans* GO3 was 4-8μg/ml. The details of the structure and *in-vitro* bioactivity of AV2010-39 will be revealed.

PP - 068

Poster Presentations

Synthesis and pharmacological evaluation of thiazolidin-2,4-diones bearing oxadiazole moiety

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ABSTRACT

The present work involves the synthesis of 5-benzyliden-3-[5-(2-benzylsulfanyl-pyridin-3-yl)-[1,3,4]oxadiazol-2-ylmethyl]-thiazolidin-2,4-diones 8a-j. The final compounds have been synthesized by condensation of 6-[3-(5-bromomethyl-[1,3,4]oxadiazol-2-yl)-pyridin-4-ylmethyl]-cyclohexa-2,4-dienethione with 5-benzylidene-thiazolidine-2,4-diones 2a-j. The synthesized compounds were screened for antitubercular, antifungal and antibacterial activities. The structures of title compounds were established by elemental, IR and ^{1}H-NMR spectral data

PP - 069

Synthesis of 1,3,4-oxadiazoles from quinoxaline and evaluation of their antimicrobial and antitubercular activities

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ABSTRACT

In this study, a new series of 5-(quinoxalin-2yloxymethyl)-2-[2-(substituted-phenyl)-vinyl]-1,3,4-oxadiazoles 5a-o were synthesized from 5-(quinoxalin-2yloxymethyl)-2-methyl-1,3,4-oxadiazole with substituted aldehydes a-o. The structures of compounds were established by spectral data IR, ^{1}H NMR and ^{13}C NMR. All the Newly synthesized compounds were screened for their antimicrobial and antitubercular activities.

PP - 070

Poster Presentations

Synthesis and characterization of some fused quinazolinone derivatives with β-lactam

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ABSTRACT

Heterocycles are important chemical entities whose deployment in pharmaceutical research resulted in myriad applications in medicine and food over past few decades. Chloroacetyl chloride is a versatile reagent and it has been extensively used in organic syntheses. It is primarily used as an acylating agent. The multi-functional nature of ClCH2COCl has made it a suitable two-carbon building block for cyclization. It is also a valuable precursor for monochloroketene and occasionally serves as a chlorinating agent. In the present context, we have incorporated well known organic synthon thiourea with another potential moiety 4-quinazolinone (which is obtained from the reaction of anthranilic acid with benzoyl chloride in the presence of pyridine) to augment medicinal value of the compound, Medicinally it has been used in various areas especially as an anti-malarial agent and in cancer treatment, after that the resultant product was treated with aromatic aldehyde, the hydrazone derivatives have been obtained, these hydrazones finally reacted with chloroacetyl chloride to give β-lactams .The beta-lactam ring is part of the structure of several antibiotic families, the principal ones being the penicillin's, cephalosporin's, carbapenems, and monobactams, which are, therefore, also called β-lactam antibiotics. These abovesaid lactams have a lethal effect on bacteria, especially on Gram-positive ones.

PP - 071

Poster Presentations

Design and synthesis of pharmacologically active benzothiazepines

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ABSTRACT

In this study we have synthesized 1,3,4-oxadiazole clubbed benzothiazepines. Benzothiazepines were synthesized by the cyclization of chalcones and finally coupled with 1,3,4-oxadiazoles. Antimicrobial activity and structure activity relationships have been studied against *Mycobacterium tuberculosis* with other pathogens. Compounds follow the Lipinski rule with few exceptions.

PP - 072

Synthesis and microbial screening of new 1,3-oxazolyl-6-iodoquinazolin-4(3*H*)ones of 2-[2-(2,6-dichlorophenyl)amino]phenyl acetic acid

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ABSTRACT

Synthesis and antimicrobial activity of 2-[2-(2,6-dichlorophenyl)amino]phenylmethyl-3-{4[(substituted phenyl)amino]-1,3-oxazol-2-yl}-]-6-iodoquinazolin-4(3*H*)ones Va-o have been reported from the parent molecule 2-[(2,6-dichlorophenyl)amino] phenyl acetic acid I, via carboxamide IV; with cyclization of substituted phenyl acetamide a-o. They were characterized and screened for antibacterial and antifungal activity at two concentrations and compared with the standard drugs. compounds V_b, V_d, V_e and V_n showed good activity.

PP - 073

Poster Presentations

Pharmacological evaluation of newly synthesized thiazolidinedione derivatives

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ABSTRACT

In attempt to make significant pharmacologically active molecule, we report here the synthesis and *in vitro* antimycobacterial and antimicrobial activity of various series of 5-{4-[2-(5-ethylpyridin-2-yl)ethoxy]benzylidine}-3-substitutedacetyl-1,3-thiazolidin-2,4-dione. The structures of title compounds were established by elemental, IR, ^{1}H NMR, ^{13}C NMR and Mass spectral data. The antitubercular activity of title compounds were evaluated against $H_{37}Rv$ using Lowenstein-Jensen agar method and antimicrobial activity against certain bacterial and fungal strain using the broth microdilution method.

PP - 074

Synthesis and *in vitro* antimicrobrial screening of phenoxyazetidin-2-ones of 5-ethyl pyridin-2-ethanol

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ABSTRACT

A new series of Schiff base and azetidinone is described; Schiff base 4a-o were prepared from the lead molecule 4-[2-(5-ethylpyridin-2-yl)ethoxy]benzaldehyde. Azetidinones 5a-o were prepared from Schiff base and phenoxy acetic acid. The structures of the compounds were assigned on the basis of elemental analysis, IR, ^{1}H NMR and ^{13}C NMR spectral data. All the products were screened against different strains of bacteria and fungi. Most of these compounds showed better inhibitory activity in comparison to the standard drugs.

PP - 075

Poster Presentations

Solublization of some insect attractants in single and mixed miceller solution and their - physico-chemical studies

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ABSTRACT

Eugenol and methyl eugenol are major constituents of some plant essential oil which are used as active ingredients in the formulation of natural insecticides and insect attractants. Literature is available on their direct application as insecticide and insect attractant but very few literature is found on their formulation.Water based and environment friendly microemulsions were prepared from these molecules. Eugenol and methyl eugenol were solublised in different concentration of SDS, Triton X-100 and Tween-80 surfactent solutions and their different mixtures. It was observed that solublization of Eugenol was maximum (5.2% w/v) in 10% (SDS + Tween-80) mixed micellar solution and minimum (0 .25%) in 2.5 % Triton X-100 solution. The solubilization of Methyl Eugenol was found almost same as eugenol in these surfactant solutions. The effect of co-surfactant e.g n-butanol and n-propanol was studied. It was observed that solubilization of eugenol was slightly enhanced (0.1-0.5%) in presence of these co-surfactants while the solubilization of methyl eugenol increased 2-3%. The effect of sodium chloride on solubilization of these compounds were negligible. The Dynamic light scattering result shows that the particle size of water based eugenol microemulsion (10% Tx-100 solution) is maximum (7.83 nm) and minimum (1.06 nm) in 5% SDS solution. The particle size of methyl eugenol microemulsion (10% Tween 80 solution) is maximum i.e 4.41nm and minimum (1.04nm) in 5% (SDS + Tween 80) solution. The change in solubilization of these insect attractants may be due to change in size of micellar droplets. The stability of these microemulsions were checked as per standard method and it was found that these formulations are quite stable.

PP - 076

Poster Presentations

Development of environment friendly emulsifiable concentrate from basil oil and its physio - chemical studies

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ABSTRACT

Basil (Ocimum basilicum) also known as Tulsi is one of the most popular herbs. The oil extracted from its leaves and the flowering tops possesses antibacterial. antifungi, neematocide properties and act as an insecticide. Basil Oil has also marked insecticide properties against mosquitoes. Some literature is available on insecticidal activity of the oil but very few literature is seen on its formulation. 5.0 % and 10.0% environment friendly emulsifiable concentrate (EC) were developed from basil oil using different vegetable oils like soyabean oil, sunflower oil and castor oil. The screenings of biodegrable emunsifiers were done for EC formulation. It was observed that mixture of non-ionic and anionic emulsifiers gave good result in the formulation as per standared specifications of EC. All parameters of the formulations were studied and encouraging result was obtained.

PP - 077

Drug–drug interaction between metformin, enoxacin and ofloxacin

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ABSTRACT

Disturbances in blood glucose including hyperglycemia and hypoglycemia have been reported in patients treated concomitantly with quinolones and an anti-diabetic agent. Therefore, careful monitoring of blood glucose is recommended when these agents are co-administered. In the present study, interactions between metformin and different fluoroquinolones; enoxacin, ofloxacin, levofloxacin, ciprofloxacin, sparfloxacin, gatifloxacin and moxifloxacin were investigated by spectroscopic (UV, IR, ^{1}HNMR) and HPLC technique. Results suggest that interaction occurred as the *in vitro* availability of metformin was considerably reduced in presence of most of the selected quinolones. It was observed that as metformin contains primary amine group, it has the tendency to complex quinolones at their ring carbonyl and carboxylic groups respectively. It is proposed that co-administration of metformin with enoxacin, ofloxacin, levofloxacin, sparfloxacin and gatifloxacin should be avoided due to the risk of pharmacokinetic drug interactions which could impair the clinical efficacy of the drugs.

PP - 078

Poster Presentations

Microwave-assisted extraction of vasicine, a potent bronchodilator from Adhatoda vasica Linn., as an alternative to conventional extraction techniques and evaluation of its bioavailability

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ABSTRACT

Adhatoda vasica Linn. is a common shrub distributed throughout India and in Ayurveda it is commonly known as vasa. Adhatoda vasica contains major phytoconstituent vasicine, which is a bioactive pyrralazoquinazoline alkaloid. It is a potent broncho-dialator and it is an active ingredient in formulations for the treatment of acute bronchitis and bronchial asthma. Presently vasicine is extracted by conventional extraction techniques like LLE, Soxhlet extraction, but these techniques are much time consuming and require large volume of extraction solvents. This paper looks at new extraction technique called Microwave assisted extraction (MAE) to prOVide faster and more efficient extract containing vasicine. The present work standardizes the extraction of vasicine from Adhatoda vasica by using Microwave assisted extraction technique. The effect of single factors such as microwave power, microwave irradiation time, extraction solvent volume, sample size etc. are evaluated and standardized. MAE, Ultrasound assisted extraction (USAE), liquid -liqUid extraction (LLE) and Soxhlet extraction has been comparatively evaluated for their efficiency to extract the content of vasicine from leaves of Adhatoda vasica. The extracts obtained by various extraction techniques were analyzed for the content of vasicine by validated RP-HPLC method. Taking into account the extraction yield, extraction time, solvent and cost of extraction, better results were obtained by MAE (100% DW 1min at High power with minimum sample size). By applying MAE the use of organic solvents was totally eliminated. Toxicity and comparative bioavailability of the MAE extract were also evaluated on animal model. MAE thus, appears the simplest, reproducible and efficient method of extraction and it can also be applied for large commercial scale-up extraction processes. The method of MAE provides as an alternative more efficient technique to extract an important phytoconstituent like vasicine. The bioavailabilty of vasicine extracted by MAE confirms the potential of using more efficient extraction technique for cheaper source of vasicine to manufacture formulations for the management of respiratory ailments.

PP - 079

Poster Presentations

Synthesis and characterization of chitosan–nucleobase conjugates for biomedical applications

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ABSTRACT

During the past few decades, there has been increasing interest in utilization of nucleobase conjugate with various natural and synthetic biopolymers. On looking all these benefits, we are interested to modify chitosan with nucleobase and utilize for various biomedical purposes. Chitin is one of the most abundant biopolymer on biosphere as polysaccharide and found as a structural component of shrimp or crab shells and fungal mycelia. Chitosan is the deacetylation product of chitin and has different properties such as hydrophilicity, biocompatibility, low toxicity and chemically inert characteristics. It has found various applications in pharmaceutical, environmental and biotechnological. We have synthesized chitosan-nucleobase conjugate and its structure was confirmed by UV-Visible, FTIR and NMR spectroscopy. The novel chitosan-nucleobase conjugate were also evaluated by X-ray diffraction (XRD), thermo-gravimetric analysis (TGA), differential scanning calorimetry (DSC), scanning electron microscopy (SEM), fluorescence spectroscopy and biological activity. Overall, the chitosan-nucleobase conjugates open new perspectives in biomedical applications.

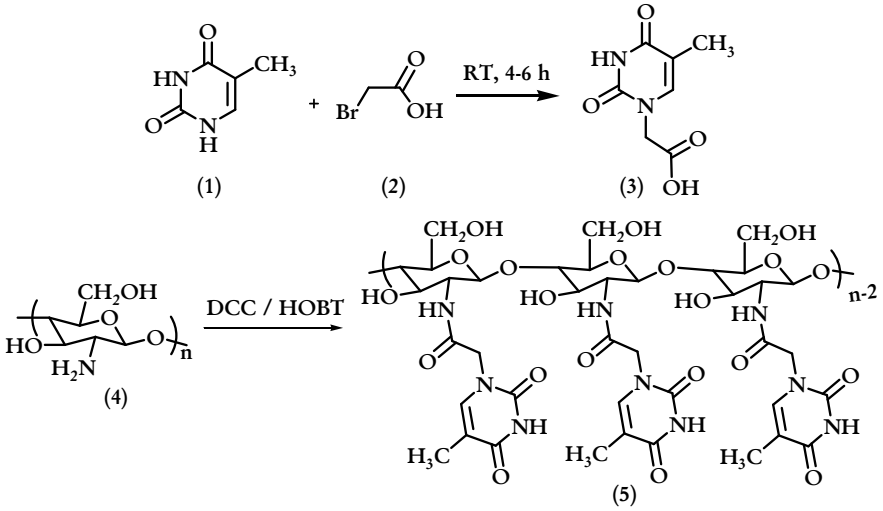

Figure 1 : Synthesis of Chitosan -Thymine conjugates

PP - 080

Poster Presentations

Asymmetric synthesis: L-proline catalyzed synthesis of homoallylic alcohols

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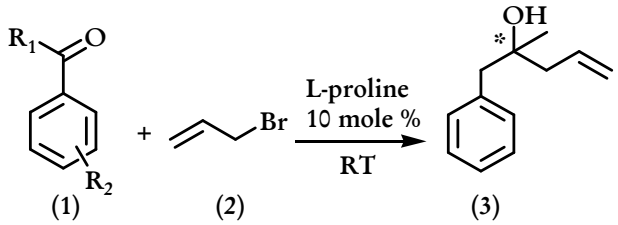
ABSTRACT

Asymmetric synthesis has become a central field in basic and applied research, especially because of the increasing necessity to avoid the formation of racemic products in chiral drug elaboration. The search for strategies that lead to the improvement and optimization of the preparation of a chiral product traditionally has included the evaluation of temperature, reaction times, addition of additives, and concentration effects, among other parameters. As one of fundamental asymmetric bond forming reactions, allyl transfer reactions from chiral reagents to the carbonyl functionality in forming enantiomerically rich homoallylic alcohols attract considerable attention from the synthetic community because the resulting products serve as chiral building block for multistep synthesis. Allylations of carbonyl compounds with allylic compounds or allyl halides are of particular interest because they are the convenient method to form C-C bond and to generate homoallylic alcohols. Catalytic asymmetric allylation of carbonyl compounds and imines is a powerful method for synthesizing enantiomerically enriched homoallylic alcohols and amines. The exceptional power of the allyllation reaction has been enhanced by newly developed enantioselective versions, especially chiral Lewis acid catalyzed allyl transfer reactions. The development of new catalytic asymmetric methods to access chiral tetra-substituted carbon-containing building blocks is an important frontier in the field of asymmetric catalysis. This method for achieving absolute stereoselection by the utilization of chiral catalysts increasingly requires precise control of the reaction pathway based on mechanistic behavior. Some amino acids and its derivatives have been used as catalyst for a long time. This amino acids have been lauded as the "simplest enzyme" due to its ability to catalyze reactions, in the last 5 years, proline has been investigated in the catalysis of reduction, oxidation. Also has been used novel catalyst for reaction like Michal addition, Mannich reaction and so. This orgno based catalyst is proved to be one of the important catalysts in the field of asymmetric synthesis. This catalyst is inexpensive and reaction can be performed under non hazardous conditions. Expanding our recent efforts on developing contemporary efficient and eco-friendly synthetic methods, herein, we report a new effective, L-proline catalyzed asymmetric allylation. In present investigation we will synthesize homoallylic alcohols from various aromatic carbonyl compounds. The asymmetric allylation of these aromatic aldehydes will be carried out using allyl bromide in presence of organocatalyst (L-Proline).



(1) (2) (3)

PP - 081

Poster Presentations

Synthesis, characterization and microbial activity of some aldimine metal complexes

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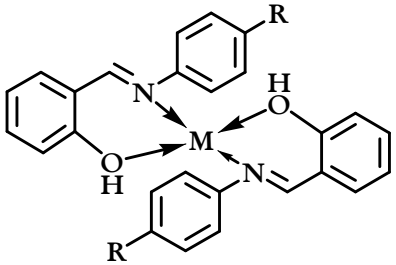
ABSTRACT

Aldimines and their metal complexes are more frequently applied for the betterment of human welfare. The importance of the Schiff base is due to the presence of >C=N- moiety. Literature survey shows that aldimines exhibit various biological activities[1-4] such as antifungal, antibacterial, antitumor, anti-inflammatory, and antipyretic etc. In the formation of complexes bidentate aldimines are superior coordinate with different metals through N and O hetero atoms. Furthermore, transition metal complexes derived from salicylaldehyde and different amines have received considerable attention because of their importance and several applications[5-8]. Applications of these metal complexes prompted us to carry out the synthesis, characterization and antimicrobial studies of some transition metal aldimines complexes. Aldimine ligand 2-Hydroxy-5-chloro-benzylidene-4-methyl-aniline and 2-Hydroxy-5-chloro-benzylidene-4-hydroxy-aniline and its complexes with Cu (II), Ni (II), Co (II) Zn (II) were prepared and characterized by analytical, spectroscopic (IR, UV-Vis) techniques, electrical conductivity, magnetic measurements and thermal study. The complexes were further screened for antibacterial activity.



ML_2 Complexes

PP - 082

Poster Presentations

Novel synthesis of some new Schiff bases as antibacterial agents

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[2]Department of Chemistry, Sharda Mahavidyalaya, Parbhani-431401, MS, India
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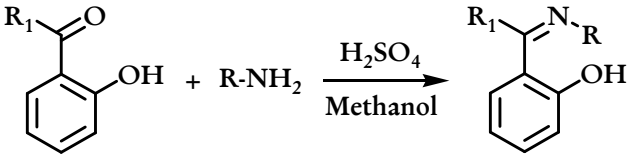
ABSTRACT

Utility of Schiff bases lies in their potent biological activity and their usefulness as a starting material for the synthesis of various heterocyclic compounds such as azetidinones and thiazolidinones. One interesting role of imines (Schiff bases) is as intermediate in the biologically important transamination reaction. Transamination is the process whereby an amino group is transferred from one molecule to another. In living systems the amino group of an amino acid is transferred to the carbonyl group of another molecule. The sequence promoted by enzyme called transaminase enzyme. The new amino acids are formed by this method. All the important transaminase enzymes appear to have common coenzymes, pyridoxal phosphate. Coenzymes are small, non-protein constituents of enzymes which are often required for enzyme activity. Schiff bases constitute one of the most active class of compounds possessing diversified biological applications. The schiff bases have been represented to posses higher degree of antitubercular and anticancer activity. The diverse and potential biological activity of Schiff bases and their enormous applications promoted us to synthesize the different new Schiff bases from 2-hydroxy aromatic ketones with aromatic, alliphatic amines and to ascertain their microbial activity.



PP - 083

Poster Presentations

Rate acceleration of baylis-hillman reaction using catalytic amount of DABCO under solvent free conditions

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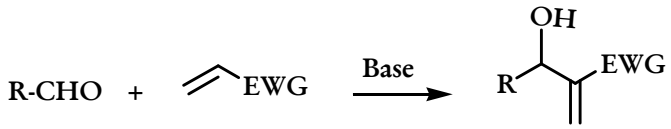
ABSTRACT

Baylis-Hillman reaction[1] is an important three step reaction involving successive Michael, Aldol, and elimination reaction in one pot. It is a reaction for carbon-carbon bond formation in organic chemistry through condensation of an aldehyde (1) to the α-position of an α-β-unsaturated system to generate a highly functionalized adduct (2) in presence of a base. (Scheme 1) This reaction is an important carbon–carbon formation process and has drawn considerable attention over the past few years. Lewis bases such as DABCO, DMAP, DBU, phosphines, chalcogen species and imidazole are frequently used in these reactions as catalysts. [2] Literature reveals that usually, the Baylis-Hillman reaction is a slow reaction requiring a few days to a few weeks for completion depending upon the reactivities of both the activated alkene and electrophile. Different group of researchers are trying to overcome the slow reaction rate in various means.[3]We are also trying to reduce the reaction rate and to improve the yield of the reaction using catalytic amount of DABCO in solvent free conditions and the details of our observation will be presented.



(1) (2)

R= alkyl,aryl EWG=CN,COR,COOR,NO_2

PP - 084

Poster Presentations

A pharmacokinetic approach to standardize β-sitosterol as a bioavailable source from linum usitatissimum seeds using high performance thin layer chromatography

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ABSTRACT

β-sitosterol is one of the key phytocontituents of seeds of Linum usitatissimum Linn. which has therapeutic action in female reproductive disorders. β-sitosterol in pure form has low bioavailability (Sarfare et al). Therefore, bioavailability and pharmacokinetic of β-sitosterol from seeds of Linum usitatissimum was evaluated using High Performance Thin Layer Chromatography (HPTLC). The study was conducted on Male albino rabbits of New Zealand strain. Blood samples were collected at different time intervals following a single oral administration of refluxed residue of Linum usitatissimum in olive oil (1g Kg-1). Absorption and elimination of β-sitosterol after administration of refluxed residue was monitored using change in the concentration of the marker band in the HPTLC profile. A marker from Linum usitatissimum seeds at RF = 0.48 was detected in rabbit plasma after half an hour of ingestion of the plant refluxed extract. The marker reached maximum concentration at 6 hrs post dose and was not detectable in plasma after 8hrs post dose. The results of this study can form baseline for making polyherbal formulation containing seeds of Linum usitatissimum to determine the pharmacological activity and bioavailability of β-sitosterol leading to a possible extrapolation to humans.

REFERENCES

[1] S Sarfare,S Menon and S Shailajan, Cornsilk as a Betasitosterol :A Pharmacokinetic study using HPTLC 9(1),2010, 44.

PP - 085

Poster Presentations

Novel synthesis of some new Schiff bases as antibacterial agents

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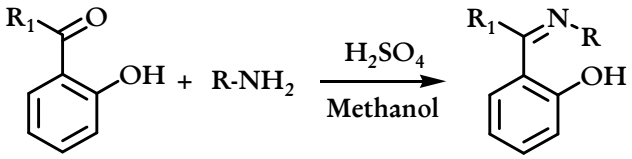
[2]Department of Chemistry, Sharda Mahavidyalaya, Parbhani-431401, MS, India
E-mail: drbrp912@rediffmail.com

ABSTRACT

Utility of Schiff bases lies in their potent biological activity and their usefulness as a starting material for the synthesis of various heterocyclic compounds such as azetidinones and thiazolidinones. One interesting role of imines (Schiff bases) is as intermediate in the biologically important transamination reaction. Transamination is the process whereby an amino group is transferred from one molecule to another. In living systems the amino group of an amino acid is transferred to the carbonyl group of another molecule. The sequence promoted by enzyme called transaminase enzyme. The new amino acids are formed by this method. All the important transaminase enzymes appear to have common coenzymes, pyridoxal phosphate. Coenzymes are small, non-protein constituents of enzymes which are often required for enzyme activity. Schiff bases constitute one of the most active class of compounds possessing diversified biological applications. The schiff bases have been represented to posses higher degree of antitubercular and anticancer activity. The diverse and potential biological activity of Schiff bases and their enormous applications promoted us to synthesize the different new Schiff bases from 2-hydroxy aromatic ketones with aromatic, alliphatic amines and to ascertain their microbial activity.



PP - 086

Poster Presentations

Pharmacophore and molecular docking based comparative study for anti tuberculosis activity with *in silico* based virtual screening

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ABSTRACT

More than 38 ligands were selected form PubChem BioAssay database for creation of ligand library which contain IC50 values (0.195-38.66 uM) for *Mycobacterium tuberculosis*. More than 80 *in vitro* anti tuberculosis positive novel heterocyclic compounds were used to generate Pharmacophore. Nine hypotheses were generated and cost value were ranges from 171.028 to 181.603. All the hypotheses had conserved features of HBA, RA except some additional features for 7 and 9 hypothes. The first hypothesis Hypo1 was characterized by highest cost (171.028), lowest RMS deviation value (1.30194) and best correlation coefficient value (0.461497). The hypothesis 1 was used to evaluate difference between each of the predicted and experimental value of the training dataset of 38 lignads. The average error in prediction was only 0.308. The fit value was observed in range of 1.04 to 2.773. Result indicated the good potential of prediction capability of the hypothesis The activity of top 20% scoring results from Pharmacophore mapping approach had *in vitro* activity in range of 32 % to 97% and 80% of ligand (18 out of 20) found have more than 60% *in vitro* activity. Similarly top 20% best scoring from GOLD docking based approach were found to have *in vitro* activity in range of 32 % to 79 %. Comparative analysis between both approach to experimentally proved *in vitro* testing displayed better performance of Pharmacophore based screening over molecular docking base screening as it was able to trap 3 best compound.

PP - 087

Poster Presentations

In silico QSAR studies of synthetic heterocyclic entities library of heterobase

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ABSTRACT

Quantitative structure-activity relationship (QSAR) is the process by which chemical structure is quantitatively correlated with a well-defined process, such as biological activity or chemical reactivity. The biological activity of molecules is usually measured in assays to establish the level of inhibition of particular signal transduction or metabolic pathways. Chemicals can also be biologically active by being toxic. Drug discovery often involves the use of QSAR to identify chemical structures that could have good inhibitory effects on specific targets and have low toxicity (non-specific activity) of special interest is the prediction of partition coefficient log *P*, which is an important measure used in identifying "drug likeness" according to Lipinski's Rule of Five. In present work *in silico* QSAR studies for drug likeness, toxicity and mutagenicity were carried out on for more than 2700 novel synthetic compounds present in the Library of Heterobase. The studies were done dragon and neural network base software for more than 30 different biological parameters. The results Generated were included into the main library of the HETEROBASE for of rapid screening of drug-like compounds for biologist and path guiding for chemist to generate new series with more compounds bearing drug like properties.

PP - 088

Poster Presentations

Novel 1-(2-picolyl)-3-benzoyl-2-benzyl-2-thiopseudourea: Synthesis, complexation with palladium and application for aqueous Suzuki reaction

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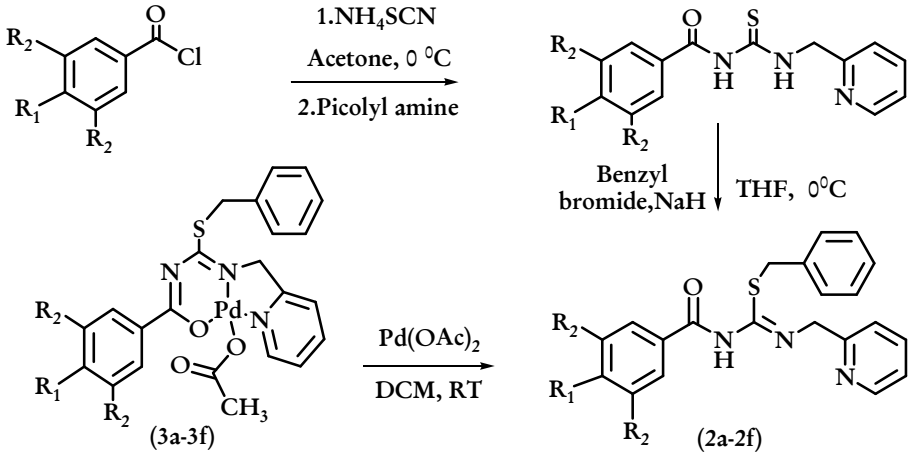
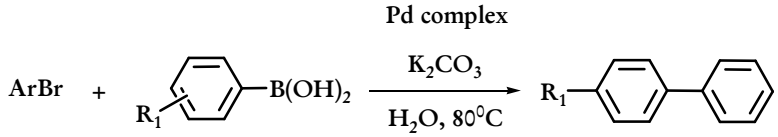
ABSTRACT

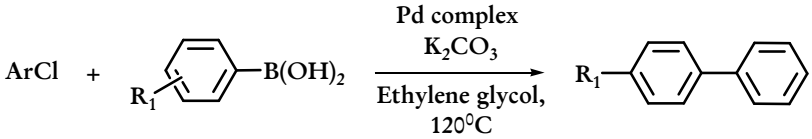
Synthesis of new ligands 1-(2-Picolyl)-3-benzoyl-2-benzyl-2-thiopseudourea and its corresponding Pd(II) complexes. The complexes have been shown to be highly efficient catalysts for Suzuki-Miyaura reaction of aryl bromides in water.



Scheme 1



Scheme 2



Scheme 3

PP - 089

Poster Presentations

Cinchona alkaloids/imidazole catalysed henry reaction of isatins: An efficient protocol for synthesis of chiral/achiral 3-substituted 3-hydroxyindol-2-ones with quaternary carbons

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ABSTRACT

The first organocatalytic, enantioselective henry reaction of isatin with nitromethane for synthesis of 3-Hydroxy-3-nitromethyl-1,3-dihydro-indol-2-one (1a) derivatives bearing C3-quaternary stereocenters were obtained in moderate to high yields (91%) and enantioselectivities (99% ee). An environmentally benign method for achiral synthesis of (1a) has also been developed starting from isatin and nitromethane in the presence of imidazole as catalyst in aqueous media.

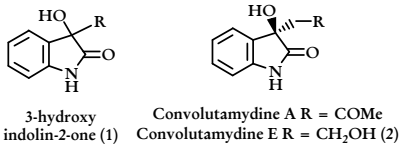
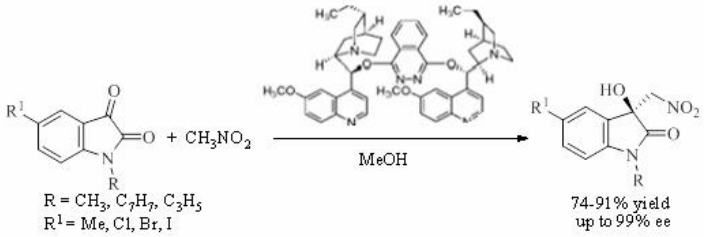
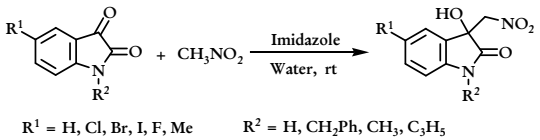


Figure 1: 3-hydroxy indolin-2-one containing natural products



Scheme 1



Scheme 2

PP - 090

Poster Presentations

Design and synthesis of azetidin-2-ones and thiazolidin-4-ones contain aryl sulfonate moiety as cox-2 inhibitors

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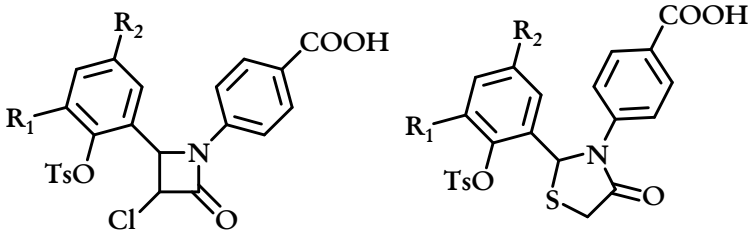
ABSTRACT

Most of the present diseases are due to the infections of pathogenic microorganisms like bacteria, fungi, and virus. The infections caused by these microorganisms posed a serious challenge to the medical community in recent years. Inflammation is the cause of many diseases and certainly a fundamental part of pain. The mechanism of anti-inflammatory drugs involves the selective inhibition of PG synthesis at the site of pain or injury. The present work demonstrates the facile synthesis of new azetidin-2-one and thiazolidin-4-one derivatives from Schiff bases containing aryl sulfonate moiety using greener methodologies. The compounds containing aryl sulfonate moiety have been received considerable attention during last two decades as they are endowed with variety of biological activities. The literature reports indicate that 2-azetidinone and 4-thiazolidinone derivatives possess different important pharmacological and biological activities such as analgesics, anti-inflammatory, anticancer, antibacterial, antitubercular, cytotoxic, and anticonvulsant activities. Keeping in view the immense biological importance of azetidin-2-one and thiazolidin-4-one derivatives, we planned to synthesize some new derivatives containing aryl sulfonate moiety and the synthesized compounds were evaluated for their anti-inflammatory activities.



PP - 091

Poster Presentations

A validated method for quantitation of Quercetin from Euphorbia hirta Linn

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ABSTRACT

Euphorbia hirta Linn commonly known as Asthma weed is found throught India and in many parts of the world. Euohorbia hirta possesses many medicinal properties such as antibacterial, anthelmintic, antiasthmatic, sedative, antispasmodic, antifertility, antifungal and antimalarial properties(Kumar et al). The plant is rich in flavanoids, triterpenoids and alkaloids. Many phytochemicals are reported in the plant such as Quercetin, Kaempferol, gallic acid, β-amyrin, β-sitosterol etc. In the current method a sensitive High Performance Thin Layer Chromatographic method has been developed for quantitation of Quercetin from Euphorbia hirta Linn. The developed method was also validated in terms of linearity, LOD, LOQ, recovery, specificity, ruggedness as per ICH guidelines.

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PP - 092

Poster Presentations

Microwave synthesis and characterization of paracetamol complexes with Co(II), Ni(II) and Cu(II)

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ABSTRACT

Novel Co(II),Ni(II) and Cu(II) complexes of paracetamol have been synthesized using microwave irradiation and conventional heating method. The microwave method was observed to be more beneficial as it provides more yield and less time consuming. Synthesized metal complexes were characterized using Infrared and electronic spectral studies. The ligand was found to be bidentiate, coordinating through the oxygen of the hydroxyl and the amide groups.

PP - 093

Preparing and characterization of Co(II), Ni(II) and Cu(II) mixed ligand complexes of pyridine, theophylline and thiocynate

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ABSTRACT

New mixed ligand complexes were prepared by adding an ethanolic solution of Theophylline (1,3 dimethyl xanthine) to an aqueous solution of metal salt. This is followed by adding a pyridine and aqueous solution of potassium thiocynate to give complexes with the general formula $[M(Tp)(Py)X_2]$ where M= Co(II),Ni(II) and Cu(II) ion,Tp=Theophylline , Py= pyridine and X=KSCN. The resulting product was found to be solid. Which have been characterized using UV-Visible spectroscopy and Infrared spectra.The present result suggested tetrahedral configuration for the metal complexes.

PP - 094

Poster Presentations

Assessment of microbial population size in the rumen of Surti buffalo (*Bubalus bubalis*): A quantitative real time PCR assay

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ABSTRACT

Traditional methods for enumerating and identifying microbial populations within the Surti rumen can be time consuming and cumbersome. In present study, a real-time PCR SYBR Green assay, using PCR primers to target total rumen microbiome of Surti buffalo (*Bubalus bubalis*) has been described. The primer sets used, were found to be target specific with no detectable cross-reactivity. Subsequently a real-time PCR approach was used to determine the population of major ruminal microbial species (Fibrolytic bacteria, Non fibrolytic bacteria, Protozoa and Methanogens) in rumen fluid of Surti buffalo fed green fodder, dry roughage and compound concentrate mixture. Among the monitored fibrolytic species, *Ruminoccucus albus* was found to be the dominant, accounting for 5.66 % of total bacteria after 24 hrs feeding. *Streptococcus bovis* and *Selenomonas ruminantium* in non-fibrolytics were detected 0.11% and 0.025% of total bacteria, respectively. Such levels of non-fibrolytics in Surti rumen suggest a synergistic relationship between fibrolytics and non-fibrolytics. Among Ciliate protozoa, *Dasytricha ruminantium* was most prevalent in the rumen, accounting 0.049 % of ciliate protozoa. Out of three orders of methanogens viz *Methanomicrobials, Methanobacterials* and *Methanococcales,* the population of *Methanomicrobials* and *Methanobacterials* was higher than *Methanococcales*, accounting 4.0% and 2.17 % respectively of total archaea.

PP - 095

Poster Presentations

Genes playing significant role for lactogenesis in buffalo

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ABSTRACT

Buffalo has been an integral part of livestock agriculture in Asia for over 5000 years producing draft power, milk, meat and hides. In the global dairy scenario India has the distinction of being the largest milk producing nation, which can be mainly credited to buffaloes for achieving and maintaining this unique status. Of the total milk production of 112 million tonnes in 2010, 55.6% came from buffalo (FAOSTAT 2010). Buffalo is a more efficient milk producer than an indigenous cow in India. In cattle several attempts were being made to understand lactogenesis process, but still it requires in-depth study as knowledge gained is insufficient. In buffalo still not such initiative is taken up. In such situation India needs to take up such study as we are harboring the world largest buffalo population. Three non-pregnant, non-lactating buffalo were induced with standard estrogen-progesterone regime. RNA was isolated from the mammary gland tissue of 0^{th}, 7^{th}, 14^{th} & 21^{st} days of induction. cDNA was synthesized for SSH and DDRT. EST's generated by modified cDNA subtraction hybridization as well as DDRT were reamplified, cloned, and sequenced. The raw sequences were analyzed using BLAST program for identifying the EST's that are playing major role during the process of induced lactogenesis. Novel EST's generated was confirmed by relative quantification.

PP - 096

Poster Presentations

Synthesis and antiinflammatory evaluation of pyrazoline derivatives

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ABSTRACT

Pyrazoline and its derivatives are a class of hetero aromatic compounds that have drawn much attention because of its biological and pharmaceutical activities like antimycobacterial, antifungal, antimalarial, antihypertensive, antihistaminic, antiinflammatory, anti- parkinson, cardiotonic, anti-cancer, antiviral and thymidylate synthatase inhibitory activities. Looking at the biological significance of pyrazoline nucleus, some novel pyrazoline derivatives were synthesized and screened for their anti-inflammatory activity. Here various substituted 2-pyrazolines were prepared by taking substituted aromatic aldehyde and substituted acetophenone in presence of NaOH for 30 min to get chalcone derivatives which was further refluxed with phenyl hydrazine (1.5 ml) in presence of pyridine for 4-6 hours with occasional shaking. The products thus formed were filtered, washed with water, dried and recrystallized from alcohol. The structures of the synthesized compounds were confirmed on the basis of UV, IR, ^{1}H NMR and Mass spectral data. The antinflammatory activity of the synthesized compounds (PYZ1-5) was evaluated by carrageenan induced paw edema method. The percentage of inhibition was calculated. Aspirin was used as reference standard. The results are statistically treated for its significance.

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PP - 097

Poster Presentations

Quality parameters of ground waters in Borsad and Anklav taluka,

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ABSTRACT

The present study deals with the Quality Parameters of Ground waters of Borsad and Anklav taluka village of Anand district of Gujarat state of India. The Ground water quality was assessed by examing various Physico-chemical parameters. Twenty-eight ground water (Borewell) samples were collected from different villages of Borsad and Anklav taluka during the month of May-2008, September- 2008, April-2009 and August-2009. The Physico-chemical parameters like Temperature, PH, TDS, DO, Total-hardness, Ca-hardness, Mg-hardness, Total alkalinity, Chloride, Sulphate, Nitrate and Phosphate have been analyzed. In the light of above results the ground water of Borsad and Anklav taluka villages, some villages are not suitable for drinking purpose. The ground water must be subjected to proper disinfect ion to ensure health of population.

PP - 098

Isolation and determination of polyvalence of bacteriophage and aantibiogram of their host bacteria

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ABSTRACT

The emergence of pathogenic bacteria resistant to most, if not all, currently available antimicrobial agents has become a critical problem in modern medicine, particularly in poultry. Improvements in biosecurity on poultry farms are likely to be very expensive and difficult to maintain, so there is a need to find an acceptable, cost effective way of preventing infection of poultry. The use of host specific bacteriophages has been promoted as a cost effective and adaptable approach to control zoontic bacteria. Twenty two fecal samples of poultry were collected from 9 different poultry farms in different districts of Gujarat. All the samples were tested for the presence of *E.coil* bacteriophage by double agar layer plaque method. The isolated phage was tested against 10 different hosts for the determination of polyvalence by cross spotting technique. Natural host has been isolated from same fecal poultry sample and their antibiogram analysis was performed. The isolated host bacteria shows high level of resistance against various antibiotics.

PP - 099

Poster Presentations

Synthesis and QSAR modelling of novel benzimidazolo thiazolidinones, thiazinones and 5-arylidene 2-imino thiazolidinones as potential antibacterial and antifungal agents

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ABSTRACT

A series of novel benzimidazolo thiazolidinones (4a-f), thiazinones (5a-b) and 5-arylidene-2-imino-4-thiazolidinones (8a-j) were synthesized and evaluated for antibacterial and antifungal activity. The compounds were synthesized in excellent yield and the structures were established on the basis of IR, ^{1}H-NMR, and their purity by elemental analysis data. All the compounds were tested for their antimicrobial and antifungal activity using Streptomycin, Penicillin and Amphotericin-B as reference drug. Many of these compounds were found to inhibit the growth of *Staphylococcus aureus* and *Escherichia coli*. Antifungal activities were evaluated against *Candida albicans* and *Rhizopus oryzae*. Some of these compounds showed potential antibacterial and antifungal activity, QSAR study was carried out using molecular descriptor derived from the 3D representation of the model with the CS Chem office version 8.0. Several types of molecular descriptor such as electronic, thermodynamic and steric have been used to derive a QSAR model between biological (antibacterial, antiviral) activity and structural properties. QSAR study reveals that the incorporation of bulky group on aryl ring may enhance the antibacterial and antiviral activity.

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PP - 100

Poster Presentations

Antioxidant activity of allylic alcohols synthesised from the sesquiterpene lactones with UHP

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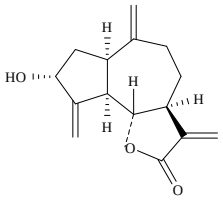
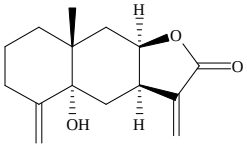
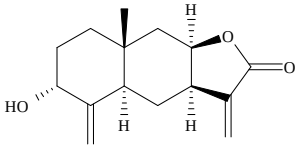
ABSTRACT

Sesquiterpene lactones like dehydrocostus lactone and isoalantolactone were subjected to allylic oxidations with selenium dioxide in combination with Urea hydrogen peroxide (UHP) replacing the common reagent TBHP to form the allylic alcohols. A further enhancement in rection rate was observed when dehydrocostus lactone and isoalantolactone were treated with SeO_2/UHP/PEG-400 under microwave irradiation. A tremendous reduction in reaction time was observed when it took only 5 minutes for the completion of reaction as compared to 4 or 5 hr under normal conditions.Moreover, the yields were higher as compared to the normal conditions. The structures of all the compounds were elucidated by spectroscopic techniques like IR,^{1}H NMR,^{13} C NMR and Mass spectra. All the compounds so obtained were subjected for toxicological evaluation. The parameters studied for toxicological behaviour include record of mortality, change in diet intake, change in body weight, change in organ weight indices, lipid peroxidation of blood and tissues and haemolysis of erythrocytes (*in vitro*). The results were fairly good over the parent compounds.







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Poster Presentations

An efficient synthesis of β-amino ketone through three component mannich reaction catalysed by anhydrous ferric sulphate

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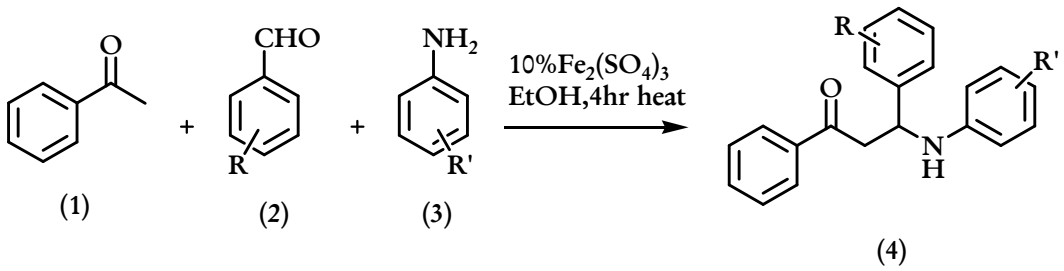
ABSTRACT

The mannich-type reactions are very important carbon-carbon bond forming reactions in organic synthesis and one of the most widely utilized chemical transformation for the construction of nitrogenous molecules[1]. In this transformation, three components, a ketone an aldehyde and an amine, react to form a β-amino ketones, which in turn are important synthetic intermediates for various pharmaceutical and natural products[2]. The increasing popularity of the mannich reaction has been fueled by the unbiquitous nature of nitrogen in drugs and natural products as well as by the potential of this multi component reaction to generate diversity. Both direct variants with unmodified ketone donors and indirect variants utilizing preformed enolate equivalents have been described[1]. In addition the imine intermediate may be preformed or its amine and aldehyde precursors used directly. Recently, direct Mannich reactions of aldehyde, ketones and aryl amines have been realized via organic and mineral acids like praline[3-5], acetic acid[6] p-dodecyl benzene sulfonic acid[7] and some Lewis acid[8,9]. They often suffer from the drawbacks of long reaction times and harsh reaction conditions, toxicity and difficulty in product separation, which limit its use in the synthesis of complex molecules. Hence, there is high interest in developing convenient methods for the synthesis of β-amino ketones. Various β-amino ketones may be synthesized through a three component reaction of ketones, aldehydes and amines catalyzed by ferric sulphate in ethanol. High yields were achieved compared with other synthetic method. This new method has the advantages of short reaction time (4 hrs), high yields, easy workup, convenient, cheap and eco-friendly.



(1) (2) (3) (4)

PP - 102

Poster Presentations

Design, synthesis, and biological evaluation of novel water-soluble *N*-mustards as potential anticancer agents

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ABSTRACT

A series of novel water-soluble DNA alkylating *N*-mustard derivatives, in which the phenyl *N*-mustard pharmacophore is attached to a benzene ring via a urea linker were synthesized. The benzene moiety contains various hydrophilic side chains are linked to the *meta*- or *para*-position of the urea linker via a carboxamide or an ether linkage. T The result revealed that these agents exhibit potent antiproliferative activity against human leukemia (CCRF-CEM) and various solid tumors cell growths in vitro. Detailed structure-activity relation studies revealed that the types of the hydrophilic side-chain (carboxamide or ether) linked to the benzene ring does not greatly affect their cytotoxicities. The selected compounds were subjected to evaluate their therapeutic efficacy in nude mice bearing human tumor xenografts. Complete tumor remission of human breast carcinoma MX-1 xenograft and significant suppression of various solid tumors were observed in animal model when treated with these derivatives. Mechanistic studies revealed that these agents are capable of inducing DNA cross-linking formation. A pharmacokinetic profile of the representative compound in rats was also investigated. The chemical synthesis as well as antitumor activity of these conjugates will be presented.

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Poster Presentations

"Curry leaves" a common indian spice, in the management of hyperlipidemia

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ABSTRACT

Hyperlipidemia is an elevation of lipids in the blood stream and including fats, fatty acids, cholesterol, cholesterol esters, phospholipids and triglycerides. It is also denoted as a major cause of atherosclerosis and coronary heart diseases. Epidemiological studies have clearly shown that the diet rich in plant foods protects human against degenerative diseases such as cardiovascular diseases. Curry leaves, (Murraya koenigii), most common Indian spice is popularly used in curries as well as in many other dishes to add spice. Besides being used as a spice, it has numerous medicinal properties like antidiabetic, antioxidant, antimicrobial, anti-inflammatory, hepatoprotective action. The current investigation focuses attention on the lipid lowering property of Murraya koenigii leaves on Triton WR-1339 induced hyperlipidemia in rats. The phytochemical fingreprint of dichloromethane extract of Murraya koenigii leaves collected from different regions was developed by using NP-HPLC on Silica column. The potentially efficacious dose of Murraya koenigii leaves with reference to the modern lipid lowering formulation (Atorvastatin) was first decided by a comparative efficacy study with three different dose groups; 250 mg/kg, 500 mg/kg and 1000 mg/kg. The current work provides the baseline data for identifying the regional variation among various samples from different regions. The significant reduced ($p = 0.05$) levels of plasma lipids in hyperlipidemic rats after treatment with Murraya koenigii leaves provide evidence for the hypolipidemic effect of Murraya koenigii. Histopathological evaluation of liver tissue also supports the lipid lowering effect of Murraya koenigii leaves. Comparable dose of Murraya koenigii leaves and Atorvastatin as evaluated proves that Murraya koenigii can be used as a combination therapy in managing formulation.

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Poster Presentations

Dimeric benzopyrans as integrase inhibitors against HIV-I and HIV–II

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ABSTRACT

The structure of a large number of HIV – integrase inhibitors have identified as two aryl units separated by a central linker. The dimeric coumarins also possess such properties. In view of this in the present paper, efforts were put in to include the phenyl ring in the 'horizontal' coumarin dimers and also the effect of electron donating or withdrawing groups were studied. Thus, 3 – [Substituted aryl/heteroaryl] - (Substituted 4 – hydroxy-2-oxo-2H-chromene-3-Yl) methyl]-substituted 4-hydroxy-2H-chromen-2-one were synthesized by known methods. The suppression of activity due to changes in the benzenoid part of coumarin skeleton seems to be noteworthy.EC_{50}, EC_{90}, and CC_{50} values of the title compounds were studied against HIV-I and HIV-II. The structures were confirmed on the basis of IR, NMR and mass spectral analysis.

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Preparing and characterization of Co(II),Ni(II) and Cu(II) mixed ligand complexes of pyridine, theophylline and thiocynate

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ABSTRACT

New mixed ligand complexes were prepared by adding an ethanolic solution of Theophylline (1,3 dimethyl xanthine) to an aqueous solution of metal salt. This is followed by adding a pyridine and aqueous solution of potassium thiocynate to give complexes with the general formula [M(Tp)(Py)X_2] where M= Co(II),Ni(II) and Cu(II) ion, Tp=Theophylline, Py= pyridine and X=KSCN. The resulting product was found to be solid. Which have been characterized using UV-Visible spectroscopy and Infrared spectra.The present result suggested tetrahedral configuration for the metal complexes.

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Poster Presentations

Synthesis of potentially useful chemotherapeutic agents derived from 1, 4 banzodiazepine class of privileged medicinal scaffolds

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ABSTRACT

On account of the wide range of the biological properties displayed by benzodiazepine derived compounds, benzodiazepine scaffold have been considered among the most important privileged structures for drug discovery. The development of novel biological materials based on the privileged structure is an intense area of research. Global efforts are underway to develop chemotherapeutic agents from 1,4 benzodiazepine class of compounds that have antiviral activity specially against human immunodeficiency [HIV] virus. The advent of HIV protease inhibitors from 1,4 benzodiazepines was hailed as a major step forward in the battle against [HIV/AIDS]. Earlier efforts directed towards the development of antiviral and anti -HIV agents from isatin and pyrimidine derivatives were found to be highly encouraging .Interestingly the incorporation of isatin with a variety of substituted amino pyrimidinyl derivatives showed an incredible potency enhancing effect in both enzymes and antiviral assays .A recent work on these compounds identified several amino pyrimidino imino isatin analogues exhibiting a broad spectrum of chemotherapeutic activity in combating HIV and OIS[the opportunististic infections like T.B.,viral ,fungal, protozoal,and neoplastic diseases] From this study compounds containing isatin ,pyrimidine , piperazine ,quinoline etc. emerged as the potent broad spectrum anti-HIV agents. Inspired by the interesting finding on the pharmacological properties of the molecules derived from isatin ,we intended in the present work to substitute the pyrimidine scaffold with the one which was active anti-HIV prone 1,4 benzodiazepine nucleus. The incorporation of isatin molecule containing the Mannich's base fragment to the 1,4 benzodiazepine nucleus was considered worthwhile to generate lead structures, as the molecular probes for anti-HIV activity.

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Poster Presentations

A facile and low solvent synthesis of hydroxyl benzyl alcohols using sodium borohydride-ammonium carbonate as reducing system

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ABSTRACT

Hydroxyl benzyl alcohols (abbreviated customarily as HBA's) are the biological relevant molecules due to their excellent neuroprotective effect[1,2] and free radical scavenging ability[3,4]. Amoong HBA's, 4-HBA is able to suppress production of nitric oxide (NO) and expression of inducible nitric oxide synthase (iNOS) in lipopolysaccharide (LPS)-activated RAW264.7 macrophages. In the macrophages, the level of reactive oxygen species (ROS) was diminished by 4-HBA. Thus, HBA's possesses anti-angiogenic, anti-inflammatory and anti-nociceptive activity possibly via its down-regulating activity on NO production, which may be partly responsible for the pharmacological efficacy of several folkloric medicines[5]. An important goal in the preparation of relevant organic compounds is the improvement of synthetic efficiency[6]. Moreover, other essential issues such as economical advantages, preservation of our resources, and care of environment, have generated a need for paradigm shift to perform chemical reactions by using ecological safe, inexpensive reagents. A general way to improve synthetic efficiency and also to address the other criteria is the development of multicomponent reactions[7]. In this regard, an efficient, high purity method amenable to the industrial scale manufacture of HBA's is reported. This synthetic protocol illustrates the preparation of HBA's by the reduction of aldehydes to the corresponding alcohols using sodium borohydride and ammonium carbonate as simple reducing system. This reaction is mild, environmentally benign, and has been of interest in process chemistry exhibiting the potential of scaling up.

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Poster Presentations

Synthesis, antimicrobial evaluation of novel fluorescent 4-(1,3-benzoxazol-2-yl)-2-phenylnaphtho[1,2-*d*][1,3]oxazole derivatives

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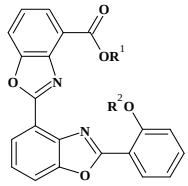
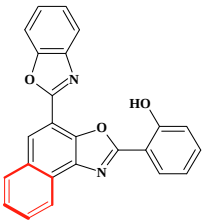
ABSTRACT

Naphthoxazoles and benzoxazoles are very important class of heterocyclic compounds because of their wide spectrum of biological and photochromatic activity. Benzoxazolyl derivatives are known for their interesting biological activity like antiviral[1], anticancer[2] antibacterial UK-1[3] since long back. They also have excellent optical properties like broad spectral windows, high molar absorptivity and fluorescence quantum yields. Some of the derivatives have been described as fluorescent probes and sensing materials, namely as fluorescent and colorimetric sensors for metals, anionic species[4]. Here, in this paper we have reported the synthesis and photophysical properties of 4-(1,3-benzoxazol-2-naphthalenol was obtained from 3-hydroxynaphthalene-2-carboxylic acid and *o*-amino phenol by successive reactions viz, oxazole synthesis followed by formation of the azo dye, 1-(4-sulphophenylazo)-3-benzoxazo;yl-2-naphthalenol, and reduction by sodium dithionate. Finally the fluorescent benzoxazolyl-naphthoxazole derivatives were synthesized by reaction with aromatic aldeydes and aromatic carboxylic acids. All these compounds were characterized by FT-IR, ^{1}H NMR, MS and elemental analyses. The synthesized compounds are fluorescent, shows dual absorption and emission pattern. All compounds were evaluated for in vitro antibacterial activities against *E. coli* and *S. aureus* strains and in vitro antifungal activity against *C. albicans* and *A. niger* strains by using serial dilution method.



UK-1 (R^1 = Me, R^2 = H)
MUK-1 (R^1 = Me, R^2 = Me)
DMUK-1 (R^1 = H, R^2 = H)



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Poster Presentations

Base-mediated regioselective intermolecular addition of alkynes to *N*-heterocycles

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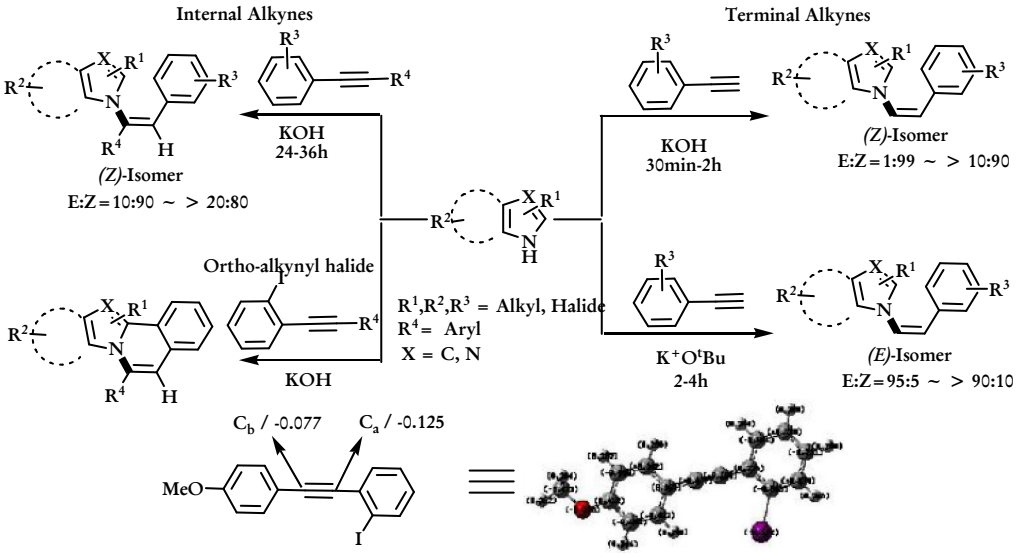
ABSTRACT

Hydroamination of alkenes, alkynes, and related unsaturated substrates represents an attractive strategy for the construction of nitrogen-containing compounds that almost prevents the formation of by-products in the creation of a C-N linkage[1]. In 1999, Knochel et al. reported the addition of phenylacetylene to heterocyclic amines in the presence of catalytic amounts of $CsOH.H_2O$ in NMP[2]. On the other hand, Kondo has reported the addition of *O*- and *N*-nucleophiles to diphenylacetylene catalyzed by metal-free phosphazene base[3]. In continuation of our interest in alkyne chemistry[4] and recently developed method for tandem synthesis of indolo- and pyrrolo[2,1-*a*]isoquinolines[5], our research plan was to find a simple and an efficient protocol for the hydroamination of alkynes. The present strategy provides a new one-step protocol for the regioselective synthesis of a wide array of (*Z*)-styryl and vinyl-enamines using KOH. Formation of (*Z*)-isomer and rate of its conversion to more stable (*E*)-product was found to be dependent on time, as well as on the choice of base. Addition of nucleophile to unactivated unsymmetrical alkynes is very important and attack on more electrophillic carbon and formation of major isomer was confirmed through DFT-B3LYP/6-31+G* calculations using Gausian 03 software[6] and by formation of cyclic indolo and pyrrolo [2,1-*a*] isoquinolines[5].



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Poster Presentations

Iodine-mediated solvent-controlled selective electrophilic cyclization and oxidative esterification of *ortho*-alkynyl aldehydes

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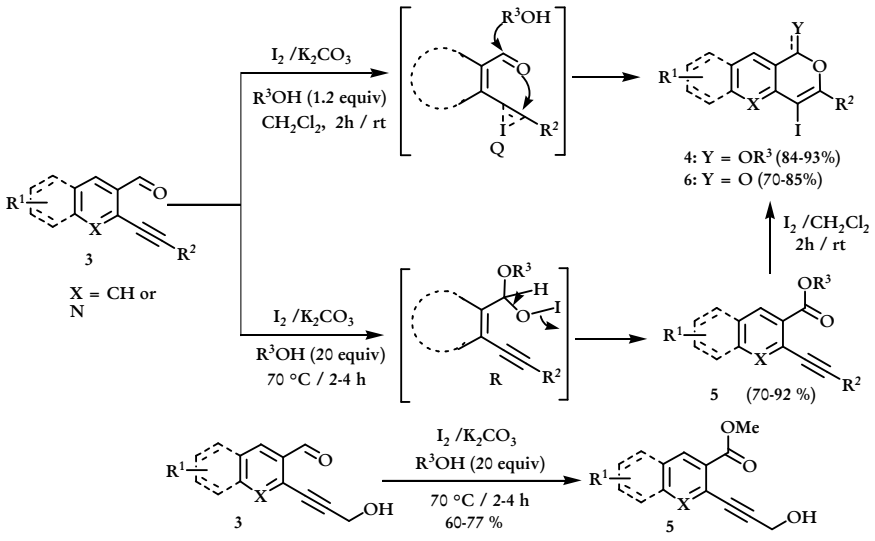
ABSTRACT

Chemoselective behaviour of iodine in different solvents in the electrophilic iodocyclization of *ortho*-alkynyl aldehydes is described. *Ortho*-alkynyl aldehydes, 3 on reaction with I_2 in CH_2Cl_2 with appropriate nucleophiles provides pyrano[4,3-*b*]quinolines 4, via formation of cyclic iodonium intermediate Q, however using alcohols as a solvent as well as nucleophile, *ortho*-alkynyl esters 2, were obtained selectively in good to excellent yields via formation of hypoiodide intermediate. Subsequently, *ortho*-alkynyl esters were converted in to pyranoquinolinones 6 by the electrophilic iodocyclization[1]. This developed oxidative esterification provides a novel access for the chemoselective synthesis of esters 5 from aldehydes 3 without oxidizing primary alcohol present in the substrate[2]. The alkaloids similar to pyranoquinolines have been reported for their interesting pharmacological as well as biological properties[3]. The halogen containing pyranoquinolines 4 and 6 are of significant interest as halogen atoms play a pivotal role in a compound's bioactivity, and such compounds provide a further avenue for structural elaboration using palladium-catalyzed reactions[4].



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Poster Presentations

In silico design of balanced dual TPR / COX antagonists

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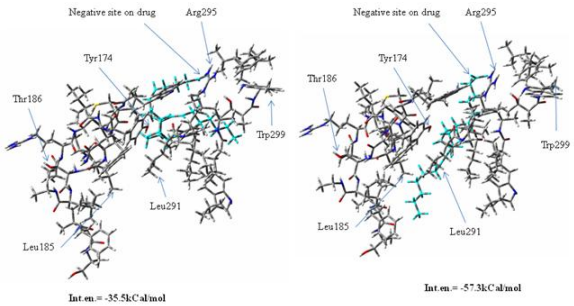
ABSTRACT

Cyclo-oxygenase (COX) enzyme catalyzes synthesis of prostaglandins and thromboxane A_2 (TxA_2). TxA_2 induces platelet aggregation and constriction of smooth muscles of vascular and respiratory origin. TxA_2 induces platelet aggregation and constriction of smooth muscles of vascular and respiratory origin. TxA_2 is considered to be one of the causes of thrombosis, asthma, ischemia and myocardial infarction. Drug discovery today utilizes the concept of multi target drug designing to achieve beneficial synergistic effects and reduce side effects. Present study is focused at in silico design of dual thromboxane receptor (TPR) / COX antagonists as drugs to avoid thromboembolism and related cardiovascular diseases. Docking studies and accurate quantum mechanical evaluation of drug-receptor interaction energies have been performed for TPR antagonists and agonists. Study highlights the thin line that separates TxA_2 antagonists from agonists in terms of specific interactions. Docking studies have also been performed for COX-2 inhibitors to understand their interactions with enzyme active site. Based on understanding of interactions of TPR antagonists with TPR binding site and COX-2 inhibitors with COX active site; an attempt has been made to design a dual TPR/COX antagonist which is balanced and shows equal activity at both leading to synergistic effects. To avoid side effects it is important for the compound to undergo 'balanced' dual inhibition. Designed compound has been derived from one of the components of a natural product and is expected to show moderate bioavailability in conformity with Lipinski's rule.



Best docking results for U-44069

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Poster Presentations

A versatile synthesis of tetrazole tethered β-carbolines via ugi- 4CC reactions

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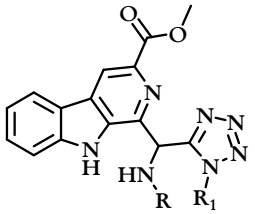
ABSTRACT

The β-carboline structural motif is found abundantly in bioactive alkaloids. Usually the β-carboline alkaloids structure is composed of two parts, which are equally responsible for their bioactivity. The main part is 9H-pyrido [3,4-b] indole and other part is tail which is composed of heterocycles, as in Manzamine alkaloids[1], Quassidines A-D[2], Eudistomin I[3], Gesashidine A[4], annomontine[5]. Multicomponent reaction (MCR) chemistry is a technique that allows for efficient and diverse access to multiple bioactive scaffolds[6]. This technique recently led to multiple biological active compounds currently undergoing clinical evaluation or even being marketed[7]. As part of our ongoing program to identify new and efficient access to scaffolds of biological interest, herein we have synthesized new β –carbolines with tethered tetrazole, for the first time using ugi 4CC reactions.



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Poster Presentations

A microwave assisted synthesis of fused lactam[1,2-a][1,4]benzodiazapine derivative by sequential ugi/coupling reaction

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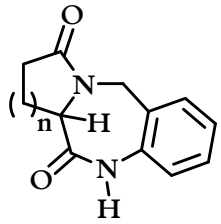
ABSTRACT

The 1,4-benzodiazepines are a noteworthy class of compounds with effective muscle relaxant[1], anticonvulsant[2], anti seizure activity[3] and sedative-hypnotic activity. Among the previously reported methods towards the synthesis of 1,4-benzodiazepine derivatives, isocyanide based multicomponent reactions are mainly important[4]. An efficient method involving Ugi 4CC followed by Cu catalyzed intramolecular coupling reaction is described herein for the preparation of fused lactam[1,2-a][1,4]benzodiazapine scaffolds. Microwave heating was used to accelerate and to improve the efficiency of the Ugi 4CC and intramolecular coupling reaction[5,6].



General structure of Ugi–coupling sequence.

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Poster Presentations

Design and synthesis of the hybrid quinazolinone-triazine as antileishmanial agents

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ABSTRACT

Leishmaniasis, caused by different species of genus Leishmania a protozoal parasite, represents a spectrum of disease have an overwhelming impact on public health throughout the world particularly in the tropics and subtropics[1,2]. Chemotherapy of patients with Leishmaniasis is a serious problem due to limited treatment options and drug resistance. Recently amphotericin B, pentamidine, and miltefosin have been discovered as effective antileishmanial drugs however all these drugs associated with the problem of serious side effects[3]. Therefore development of less toxic drugs based on new molecular scaffold that are effective against all forms of leishmaniasis is urgently needed. A great number of natural and synthetic compounds comprising divergent chemical structures have been tested in the past few years in antileishmanial assays and among these, quinazoline class of compounds have been reported to possess antiprotozoal activities through DHFR inhibition[4]. While on the other side triazine class of compounds being the inhibitors of DHFR have also been identified as potential antileishmanial agents[5]. Based on these observations we have designed and synthesized the hybrids of quinazolinone with 1,3,5-triazine and screened for their antileishmanial profile. The encouraging results have been obtained and further biological studies of these compounds are currently underway.

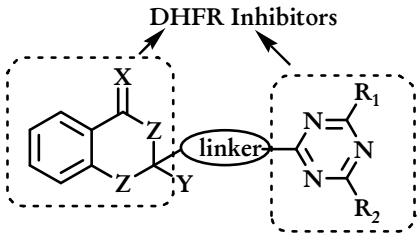

Figure 1: Hybrid of Quinazolinone-triazine

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Poster Presentations

Design and synthesis of new chalcone derivatives containing triazine moiety with potent antitubercular activity

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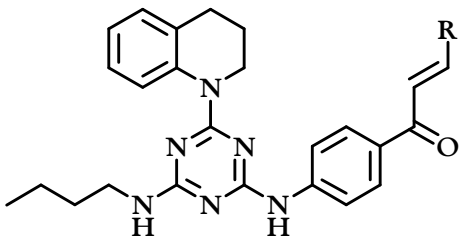
ABSTRACT

Tuberculosis (the contagious airborne disease) is one of the leading infectious diseases, remains a major global health problem and reemerged as a serious health threat, fueled by the spread of multidrug-resistant (MDR) strains. From WHO reports in 2006 nearly one -third of world population is infected with Mtb, resulting 1.7 million deaths worldwide. Treatment of Tuberculosis in conjunction with HIV becomes more challenging, needs long and costly treatment. In current, the DOTS Therapy is applying for treatment of Mtb. Which needs 6 to12 month periods and high cost[2]. Poor chemotherapeutics and the inadequate administration of drugs have led to the development of multidrug resistant TB (MDR-TB), the treatment of which requires administration of more expensive, second line antibiotics for up to 2 years. In addition, even more alarming cases of extensively drug resistant strains of TB (XDR-TB) that are resistant to both first and second line drugs have been reported[3]. Chalcones are essential intermediate compounds in flavonoid biosynthesis in plants and showed various biological properties of natural and synthetic chalcones. Chalcones are also cited as being antibacterial, including *M. tuberculosis*, by Lin et al.,[4] however; no information on the target of action of the compounds is available. On the other hand Dihydrofolate reductase (DHFR) is a key enzyme of folate biocycle and also a prime target for infectious diseases[5]. So keeping this view in mind we synthesized the triazinyl chalcones as antitubercular agents. Biological activity of the synthesized compounds is under progress.



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Poster Presentations

Synthesis and anti-microbial activity evaluation of novel dithiocarbamate-aminoquinoline/pyridine conjugates

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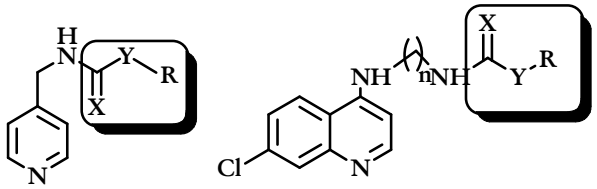
ABSTRACT

Microbial infections are still the most serious threats to immune compromised patients. Currently available drugs for treatment of microbial infections are limited. An anti-microbial is a substance that kills or inhibits the growth of microorganisms such as bacteria, fungi, or protozoan's. Anti-microbial drugs either kill microbes (microbiocidal) or prevent the growth of microbes (microbiostatic)[1]. Substituted dithiocarbamic acid esters are a common class of organic molecules. The different derivatives in this group exhibit a wide range of biological effects (antibacterial, antifungal, antioxidant activity, inhibition of cardiac hypertrophy, etc.)[2]. In addtition, quinoline and pyridine moieties are of great importance to chemists as well as biologists as it is found in a large variety of naturally occurring compounds and also chemically useful molecules having diverse biological activities. Amongst the various activities of their derivatives, anti-microbial activity is noteworthy. It is interesting to note that quinoline is a core pharmacophore in the recently developed anti-tuberculosis drugs, viz. TMC207, a diarylquinoline (DARQ), mefloquine, and moxifloxacin[3]. Due to continuous increasing of antibacterial resistance in hospital and community settings and reducing treatment options for patients thus there is need to active research efforts aimed at developing new antibacterial agents to treat resistant bacterial pathogens[4]. Therefore for the development of new antimicrobial agents, we synthesize a series of novel dithiocarbamate-aminoquinoline/pyridine analogues. Biological screening against *M. tuberculosis* is under progress.



MIC: 1.56 mg/mL **MIC: 1.56 mg/mL**

Figure 1: Activity against candida albicians, cryptococcus neoformans, candida parapsilosis

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Poster Presentations

Synthesis of new 4-aminoquinoline-schiff base derivatives as potent antimalarial agents

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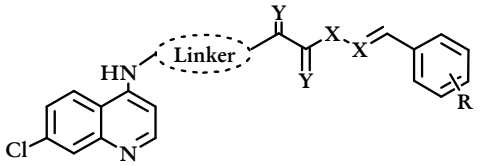
ABSTRACT

Malaria, a tropical, re-emerging infectious disease, has been a primary concern to humanity for centuries and is now extended to more than 40% of the world's population. Besides increasing resistance against several types of protozoan parasites of the genus *Plasmodium,* several other factors like increasing insecticide resistance of the *Anopheles* mosquito are also participating in the increasing spread of malaria[1]. Even after a tremendous development in medical science and R&D against malaria we still need new antimalarial drugs, in view of developing parasitic resistance to the commonly used ones. Design and synthesis of hybrid 4-aminoquinolines having multiple targets can be a hope of generating effective antimalarial chemotherapy[2]. The quinoline anti-malarials inhibit β-haematin formation in the parasite and subsequently lead to formation of toxic haem that kills the parasites[3]. The 4-aminoquinoline structure constitutes an interesting basis for the design of novel compounds displaying increased activity[4]. The oxalamide functionality in the side chain of 4-aminoquinoline provides stability towards enzyme degradation[5] and retained H-bonding ability[6]. Further the Schiff base chemistry is selected for introducing modifications on the 4-aminoquinoline nucleus[7]. In this perception we have synthesized one such series of 4-aminoquinolines having oxalamide and schiff base functionalities in the side chain with the aim of generating new antimalarials.



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Poster Presentations

Synthesis of amadiaquine - aplysinopsin hybrids as novel antimalarial agents

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ABSTRACT

At the border between bio-inspired and rational drug design, one can imagine preparation of hybrid molecules with a dual mode of action to create efficient new drugs. Hybrid molecules are defined as chemical entities with two or more structural domains having different biological functions and dual activity.[1] Aplysinopsin has recently been discovered as a potential antimalarial agent.[2] As a part of our ongoing research devoted for the synthesis of diverse hybrid heterocycles of amadiaquine with immense success against resistant strain of *Plasmodium falciparum*, a series of hybrid molecules containing amadiaquine and aplysinopsin has been prepared and evaluated for its antimalarial activity.

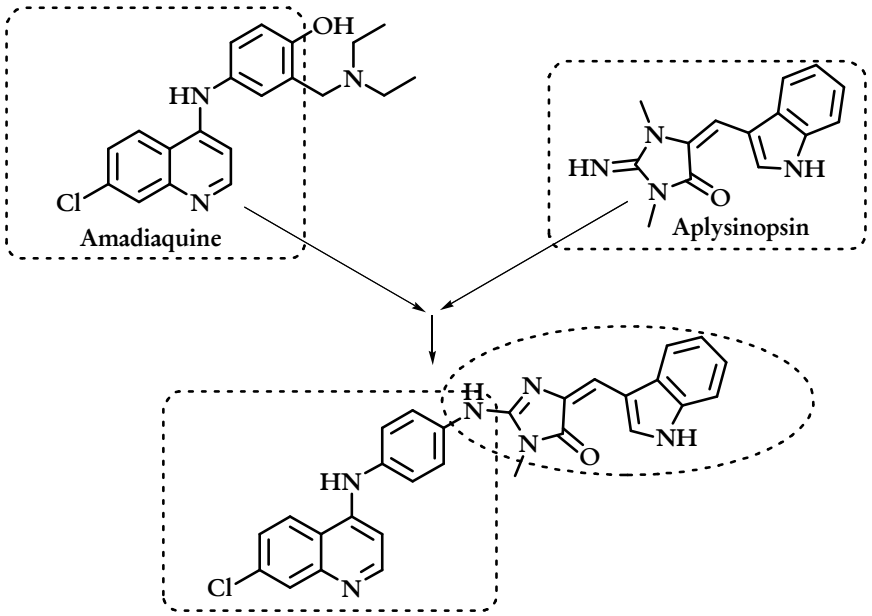

Figure 1: Amadiaquine - aplysinopsin hybrid

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Poster Presentations

Synthesis and biological evaluation of indolyl glyoxylamides as a new class of antileishmanial agents

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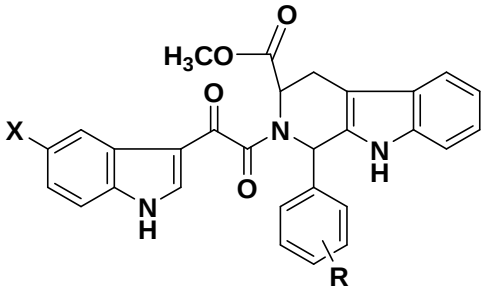
ABSTRACT

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. Leishmaniasis is a vector born parasitic disease of the tropics and subtropics which is manifested in four major clinical forms (cutaneous leishmaniasis, mucocutaneous leishmaniasis, visceral leishmaniasis, and post kala-azar dermal leishmaniasis or PKDLa) depending on the causative species of the protozoan. Among all above, visceral leishmaniasis is lethal, if left untreated. Natural and synthetic β-carbolines and tetrahydro-β-carbolines alkaloids are well-known compounds that possess a variety of biological properties. Recent studies have pointed β-carboline alkaloids as potential antileishmanial agents[1]. Earlier, we have demonstrated indolylglyoxylamide derivatives as potent antileishmanial agents[2,3]. Based on the above observations, we designed and synthesized indolylglyoxylamides of tetrahydro-β-carbolines as an entirely new structural class of indolylglyoxylamides with antileishmanial activity[4].



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Poster Presentations

Piperazine derived antispermatogenic agents as oral contraceptive for men: Design, synthesis and *in vitro* evaluation

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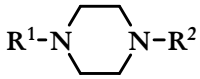
ABSTRACT

Antispermatogenic agents that reversibly interrupt spermatogenesis may have a contraceptive relevance for men[1]. N-substituted diamines (N,N‘-bisdichloroacetyl, N,N‘-diethyl-1,4-xylenediamine) have been reported as antispermatogenic agents[2]. Based on these studies it was thought worthwhile to utilise piperazine framework (an important building block in various bioactive compounds) as starting material. A series of seventeen compounds were synthesized and evaluated for *in-vitro* antispermatogenic activity using rat Sertoli cell cultures. 10 compounds exhibited significant activity with an MIC of 2.5 μM-25 μM.



R^1, R^2 = acyl, aryl, chloroacetyl, substituted acyl

Figure 1 : General structure of the synthesized compounds

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Poster Presentations

Synthesis and antihyperlipidemic activity of novel coumarin bisindole derivatives

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ABSTRACT

Cholesterol plays a major role in the assembly of membranes and performs other important biological functions in human heart health. However, when plasma cholesterol exceeds the level required for these functions, it results in the development of atherosclerotic cardiovascular disease such as coronary heart disease and stroke[1]. Hyperlipidemia may also induce other abnormalities like oxidation of free fatty acids, leading to the formation of ketone bodies as well as masking liver and muscles resistance to insulin which initiates the progress of diabetes in patients[2]. So, in continuation of our ongoing drug discovery programme, for developing new antidyslipidemic drugs[3], a series of novel coumarin bisindole heterocycles (5a–5h & 9a–9d) were synthesized following an uncommon method and evaluated for their antihyperlipidemic activity in hyperlipidemic hamster model. Among 12 compounds tested, the compound 5e showed potent antihyperlipidemic activity and was found to decrease the plasma triglyceride levels (TG) by 55%, total cholesterol (TC) by 20%, accompanied by an increase in HDL-C/TC ratio by 42% in hyperlipidemic rats to a greater degree than some of the reference standard lovastatin and atorvastatin. Initial studies indicate compound 5e to be devoid of cytotoxicity in normal cells. Furthermore, dose dependent studies on 5e done at different doses 2.5, 5, 10, and 25 mg/kg body weight, revealed that the optimum dose for compound 5e was at 10 mg/kg body weight. Compound 5e merits further detailed investigation in our continuing program to generate and develop lipid lowering agents.

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Poster Presentations

Synthesis and triglyceride lowering effect of novel benzocoumarin derivatives in hyperlipidemic hamsters

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ABSTRACT

Dyslipidemia and coagulation disturbances are among the most significant risk factors of the development of atherosclerotic condition.[1] Elevated plasma concentration of cholesterol, especially low-density lipoprotein (LDL) and triglyceride is recognized as a leading cause in the development of atherosclerosis and coronary heart disease.[2] Statins and fibrate class of drugs are the most widely used candidates for treatment of dyslipidemia. Statins (HMG-CoA reductase inhibitors) used for lowering LDL-cholesterol are pretty effective. However, most patients still experience adverse coronary events despite statin therapy. Fibrate class (PPARα agonists) of drugs, which are mostly used to treat hypertriglyceridemia and low HDL-cholesterol, requires high doses to show significant efficacy.[3] Therefore, there is a constant need for a different class of potent compounds to treat dyslipidemia without severe side effects. So in continuation of our drug discovery programme,[4] synthesis of a series of benzocoumarin - Schiff bases is reported. The novel compounds were evaluated for their antihyperlipidemic activity in hyperlipidemic hamster model. The compound 7 at a dose of 5 mg/kg body weight significantly lowered the plasma triglyceride levels (TG) by 62%, total cholesterol (TC) by 48%, accompanied by an increase in HDL-C/TC ratio by 62% in hyperlipidemic hamsters to a greater degree than some of the reference statins.

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Poster Presentations

Design and synthesis of 3-(azol-1-yl)phenylpropanes as microbicidal spermicides for prophylactic contraception

Lalit Kumar,[a] Amit Sarswat,[a] Nand Lal,[a] Ashish Jain,[b] Sumit Kumar,[a] S.T.V.S. Kiran Kumar,[a] Jagdamba P. Maikhuri,[b] Atindra K. Pandey,[c] Praveen K. Shukla,[c] Gopal Gupta[b] and Vishnu L. Sharma[a,*]

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ABSTRACT

Good reproductive health is the basis for intimate relationship, happy family and healthy children, which ensures that every child is wanted, every birth is safe, and every person is free of candidiasis, STI and HIV[1]. Therefore, developing user-friendly, self-administrable, anti-STI vaginal spermicides has become an urgent global priority[2]. So we designed a series of 25 3-(azol-1-yl)phenylpropanes which yielded 10 compounds (3,4,7,8,13,14,19,21,23,26) that irreversibly immobilized 100% human sperm at 1% (w/v) concentration in 60 seconds; twelve compounds (8,9,15,16,19-21,23-25,27,28) that showed potent microbicidal activity at 12.5-50 μg/mL against *Trichomonas vaginalis*; and 17 (3-11,13,15,19,21,23,26,28,30) that exhibited potent anticandida activity with minimum inhibitory concentration (MIC) of 12.5-50 μg/mL. Almost all the compounds exhibited high level of safety towards normal vaginal flora (*Lactobacillus*) and human cervical (HeLa) cells in comparison to the marketed spermicide nonoxynol-9 (N-9)[3]. All the biological activities were evaluated *in vitro*. Two compounds (4,8) with good safety profile exhibited multiple (spermicidal, antitrichomonas and anticandida) activities, warranting further lead optimization for furnishing a prophylactic vaginal contraceptive.

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Poster Presentations

Arylpiperazines for management of benign prostatic hyperplasia-design, synthesis and biological evaluation

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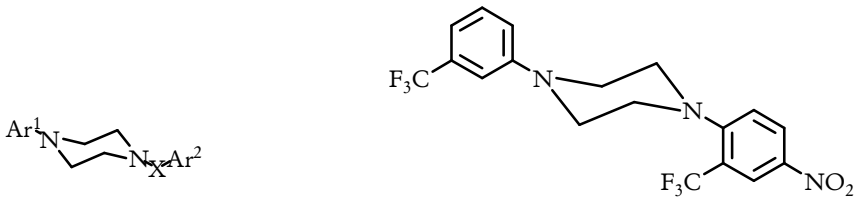
ABSTRACT

Benign prostatic hyperplasia (BPH) is an ubiquitous[1]condition in the aging males, such that the incidence of BPH detected at autopsy increases from approximately 30% at age 50 to >80% at age 80. The available treatments for BPH are either highly invasive (surgical) or partially effective with unwanted side effects. Direc. Therefore, a potent agent with fewer adverse effects is highly desirable. Recently, arylpiperazine derivatives have been reported as potent nonsteroidal AR antagonists[2]. A series of 27 aryl/heteroaryl/aralkyl/aroyl piperazines were synthesized and most of these compounds reduced prostate weight of mature rats by 15-47%. Three compounds **10**, **12** and **18** had better activity profile (reduced prostate weight by 47%, 43% and 39%, respectively) than the standard drug flutamide (24% reduction). A 10-fold decrease in PSA and 15-fold increase in ER-β gene expressions of human prostate cancer cells (LNCaP) by compound **10** *in vitro* indicated AR and ER-β mediated actions. The findings may stimulate further explorations of identified lead for the management of benign prostatic hyperplasia.



Ar1, Ar2 = aryl, X = CO, CH_2

Figure 1: General structure of synthesized compounds

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Poster Presentations

Microwave induced synthesis of azo compound: A solvent free path for some dyes

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ABSTRACT

An efficient method for the exclusive one pot synthesis of sodium salt of benzidine diazo-bis-1-naphthylamine-4-sulphonic acid (an azo compound) under condition of microwave irradiation. The reaction was found to follow diazotization and condensation mechanism with removal of water molecules. Formation of product was confirmed through TLC, M.P. and spectral analysis. The reaction was carried out in a single pot without using solvent in a domestic microwave oven.

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Synthesis of 3-acetyl and 3-acetoacetyl pyranobenzopyran as anti-HIV agents

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ABSTRACT

Coumarin nucleus recently has assumed importance for their anti-HIV potency against integrase and protease, the key enzymes responsible for viral replication, in our earlier work, we have demonstrated that coumarin possess marked antiviral activity. Recently it has been established as a lead molecule towards inhibition of HIV-I and HIV-II. The structures were confirmed on basis of IR, NMR and Mass spectra and elemental analysis.

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Poster Presentations

Enviro-economic synthesis of some phthalimide derivatives using microwave irradiation

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ABSTRACT

An environmentally benign, efficient and facile route is developed for the preparation of phthalimide derivatives by using LiBr as a catalyst under solvent free condition and microwave exposure. In comparison to conventional synthesis involving tedious workup, excessive use of solvent and extra labour for separation and purification of compounds, the present method indicates operational simplicity, shorter reaction time and higher yields which can prove this procedure as a useful alternative for the synthesis of heterocycles. The aim of present work is to synthesize medicinally important heterocyclic moieties by green chemical methodology. The synthesized compounds have been characterized by various analytical and spectral techniques. The synthesized compounds have been evaluated for their antibacterial and antifungal activities.

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Poster Presentations

Efficient synthesis of 4-aryl/alkyl-3,4, dihydro-2(1H)-pyrimidone esters and 5-acetyl-4-aryl/alkyl-6-methyl-3,4 dihydropyrimidin-2(1)-ones on montmorillonite clay modified with Zn salts

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ABSTRACT

An efficient, extremely fast and ecofriendly method for the synthesis of some dihydropyrimidines over modified montmorillonite K-10 clay (clayzin, clayzic, clayzis) under microwave irradiation has been reported. A considerable increase in the reaction rate has been observed with reasonable good yields. Modified montmorillonite K-10 acts as a solid support as well as catalyst for the synthesis of dihydropyrimidines. Substituted aldehydes, β–dicarbonyl compounds and urea (or thiourea) were used as starting materials for the synthesis of substituted 4-aryl/alkyl-3,4-dihydro-2(1H)-pyrimidone esters and 5-acetyl-4-aryl/alkyl-6-methyl-3, 4-dihydropyrimidine-2(1H)-ones.

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Poster Presentations

Photocatalytic degradation of polluted water in presence of copper hexacyaoferrate (II)

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ABSTRACT

Photo labile property of ferrocyanide ion is well knows. The electron generated by ferrocyanide ion on exposure of light may be utilized for the photoreduction of dye. In the present work use of use of photo labile nature of ferrocyanide ion was made for the photocatalytic degradation of erythrosine B dye. Copper hexacyanoferrate (II) was synthesized and used for this purpose. Effect of different parameters like pH, concentration, light intensity etc. was studied on the rate of reaction. A suitable mechanism for the phototcatalytic degradation of erythrosine B dye has been proposed.

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Occurrence and extracellular enzymatic activity profiles of bacilli strains isolated from soil

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ABSTRACT

The advances in genetics and microbial physiology have a strong impact enzyme production; screening programmes for the selection of microorganisms able to produce bioactive molecules continue to be an important aspect of biotechnology. The spore-bearing alkaliphilic Bacillus species constitute a large, heterogeneous group of microorganisms which are now being investigated in order to better understand the physiology, biochemistry and especially molecular genetics underlying the behavior of microbes. Extracellular or exoenzymes are those enzymes that are completely dissociated from the cell and found free in the surrounding medium. In the current work, extracellular enzymatic activity profiles of Bacillus strains isolated from soil of different cultivated regions have been studied. Bacillus strains were screened by using different selective media. About 80% of the isolates tested showed extracellular enzymatic activity. Out of the twenty isolates screened eight, six, five and five isolates exhibited Amylase, Nuclease, Xylanase and Cellulase activities respectively. Activity of crude enzymes was assessed by using spectrophotometric assays. The enzyme has been partially purified.

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Poster Presentations

Degradation of bismark brown-R using copper loaded neutral alumina as heterogeneous photo-fenton reagent

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ABSTRACT

In the present work, heterogeneous photo-Fenton degradation of bismark brown-R has been investigated in aqueous medium using visible light. The photocatalyst has been prepared by loading Cu^{2+} ions in neutral alumina. The rate of photocatalytic degradation of dye was monitored spectrophotometrically. The effect of variation of different parameters like pH, concentration of dye, amount of photocatalyst and light intensity on the rate of photocatalytic degradation was also observed. Photocatalyst has been characterized by inductively coupled plasma optical emission and IR spectroscopy and scanning electron microscopy. COD of the reaction mixture before and after treatment was determined A tentative mechanism for the photocatalytic degradation bismark brown-R has also been proposed.

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Poster Presentations

Synthesis, characterization and thermal degradation of p-chloroacetophenone oxime based polymers having biological activities

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ABSTRACT

A monomer p-chloroacetophenone oxime (CAO) has been prepared from p-chloroacetophenone and hydroxylamine hydrochloride. Its copolymer resin, p-chloroacetophenone oxime – formaldehyde (CAO-F) has been synthesized from p-chloroacetophenone oxime (CAO) and formaldehyde in 1:2 molar proportion. Terpolymer resins, p-chloroacetophenone oxime-formadehyde-benzoic acid (CAO-F-BA) has also been synthesized using p-chloroacetophenone oxime (CAO), benzoic acid (BA) and formaldehyde (F) in 1:1:5 molar proportions by ondensation in acid medium. The structures of monomer, copolymer and terpolymer have been investigated by FT-IR, ^{1}H NMR and pyrolysis (GC/MS) techniques. Molecular weight and polydisperity index have been determined by gel permeation chromatography. Detailed thermal degradation studies of polymers have been carried out to ascertain its thermal stability. Multiple linear regression (MLR) method has been used to calculate activation energy (E_a) and frequency factor (Z). Thermodynamic parameters such as free energy (G), entropy change (ΔS^*) and k have been evaluated on the basis of Ozawa method. Softening temperature (T_s) of these resins has been obtained from differential scanning calorimetry. All the synthesized resins have shown excellent antimicrobial activities as compared to standard drugs.

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Poster Presentations

Use of dimethyl carbonate as methylating reagent in microwave assisted reactions: a green chemical path

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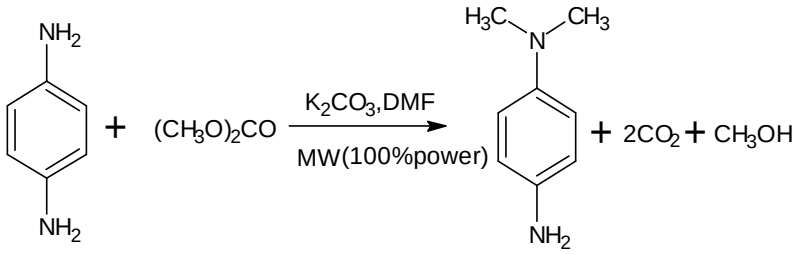
ABSTRACT

Alkylation is a very important chemical reaction which modifies the biological properties of drugs. The alkylation was optimized using dimethyl carbonate under microwave irradiations. Dimethyl carbonate is environmentally safe and less toxic methylating reagent, dimethyl carbonate (DMC), has been developed. This method provides desired products in high yields with high purity under microwave condition and is suitable for large-scale production. The effect of various functional groups on the aromatic amines has been investigated. Green material have been developed to minimize the environmental pollution problem and in the design of eco-friendly synthesis. We planned to carry out this reaction in microwave irradiation because MORE chemistry is not only eco-friendly procedure but also it reduces reaction time as compared to conventional method, ease of work up after reaction and better selectivity. The product obtained by this method was confirmed by GC-MS and other spectral data.



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PP - 134

Poster Presentations

Photocatalytic mineralisation of benzene hexachloride

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ABSTRACT

In the present work, Photo catalytic Mineralization of Benzene hexachloride using zinc oxide as semiconductor has been carried out. The progress of reaction has been monitored volumetrically using NaOH as titrant pseudo- first order kinetics has been found for the photocatalytic degradation tentative mechanism for the photocatalytic degradation of benzene hexachloride has been proposed involving OH radical.

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A comparative study on photocatalytic degradation of methylene blue by sol-gel synthesized transition metal doped tio$_2$ supported on zeolite

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ABSTRACT

Transition metals (Ni, Cr, V, Fe) modified TiO_2 loaded on zeolite, semiconductors were prepared by sol-gel method. The nanosized photocatalysts were characterized by X-ray diffraction (XRD) and Scanning electron microscopy (SEM) techniques. Their photocatalytic activities were examined by the photocatalytic decolourization of methylene blue dye under solar readiations. The rate of photocatalytic degradation was monitored spectrophotometrically. Effect of pH, dye concentration, intensity of light and amount of semiconductor on the degradation of methylene blue were primarily investigated. The results show that the doping enhances the photocatalytic activity in comparison to normal TiO_2. The order is found to be- Cr-TiO_2/zeolite > V-TiO_2/zeolite > Ni-TiO_2/zeolite > Fe-TiO_2/zeolite > TiO_2. The photocatalytic mechanism has also been discussed.

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Poster Presentations

Synthesis, characterization of hydroxyl-Fe-pillared bentonite and its use in heterogeneous photo-Fenton degradation of rose Bengal

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ABSTRACT

The degradation efficiency of rose Bengal dye in aqueous medium using hydroxyl Fe pillard bentonite as heterogeneous photo-Fenton reagent has been assessed. It was found that the heterogeneous photo-Fenton process was relatively more suitable as compared to its homogeneous counterpart. In heterogeneous system, the catalyst can be reused and the possible pollution caused by the ferrous ions in solution of homogeneous process can also be avoided. Hydroxyl-iron-pillared-bentonite was prepared through cation exchange reaction, and used as a solid catalyst for photo-Fenton process. Effect of various parameters like pH, dye concentration, amount of hydrogen peroxide, light intensity and amount of catalyst on the rate of reaction was observed. A tentative mechanism has been proposed for photo-Fenton degradation of rose bengal.

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Poster Presentations

Enhancing photocatalytic activity of zinc oxide by coating with chlorophyll

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ABSTRACT

Photocatalytic activity of zinc oxide can be enhanced by the coating of some natural pigments. In the present work zinc oxide is coated by a natural plant pigment, chlorophyll. Coated photocatalyst has been used for the photobleaching of rose bengal dye. Progress of the reaction has been monitored spectrophotometrically by measuring absorbance of the reaction mixture at definite time intervals. The effect of variation of different parameters such as pH, concentration of dye, amount of semiconductor and light intensity on the rate of photobleaching was also observed. A tentative mechanism for the reaction has been proposed.

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Poster Presentations

Sonolytic, photocatalytic and sonophotocatalytic degradation of toluidine blue

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ABSTRACT

In the case of photocatalytic oxidation, the most common problem associated is the high efficiency of the cavity and electron composition, the low efficiency of reactivity and that the catalyzer can agglomerate easily, which can be get over by sonophotocatalytic oxidation technology. This modification can improve the efficiency of wastewater treatment. This paper introduced the mechanism of sonophotocatalytic treatment of wastewater and the effects of various parameters such as pH variation, dye concentration, amount of semiconductor, and particle size of zinc oxide influencing the efficiency of wastewater treatment.

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Poster Presentations

Photocatalytic bleaching of azure-B in the presence of ammonium phosphomolybdate

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ABSTRACT

The photocatalytic degradation of azure-B has been carried over ammonium phosphomolybdate as semiconductor in the presence of light. The progress of reaction has been monitored spectrophotometically. The effect of variation of different parameters like concentration of dye, light intensity, pH, and amount of semiconductor on the rate of photocatalytic bleaching was observed. Mechanism involving $^{\bullet}OH$ radical for photocatalytic degradation of azure-B has also been proposed.

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Poster Presentations

Photochemical oxidative degradation of cresol red using potassium trisoxalatoferrate (III) as an oxidant

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ABSTRACT

The photochemical oxidative degradation of Cresol red by potassium trisoxalatoferrate (III) has been investigated. The rate of photochemical degradation of dye was observed spectrophotometrically. The effect of variation of different parameters like pH, concentration of complex and dye, amount of light intensity on the rate of photochemical degradation has also been observed. A tentative mechanism for the photochemical oxidation of Cresol red has been proposed.

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Poster Presentations

Synthesis and antimicrobial evaluation of 4-(5'-chloro-3'-methyl-1'-n-phenyl-pyrazol4'yl)-2,6-dimethyl/6-isopropyl-3,5-disubstituted phenylcarbamoyl-1,4-dihydropyrimidines

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ABSTRACT

Bacterial resistance is a major drawback in chemotherapy of infectious diseases. In this investigation a new series of 4-(5'-chloro-3'-methyl-1'-N-phenyl-pyrazol4'yl)-2,6-dimethyl/6-isopropyl-3,5-disubstituted phenylcarbamoyl-1,4-dihydropyrimidines (I_{a-t}) have been synthesized by the cyclo- condensation of 5-chloro-3-methyl-1-phenyl-pyrazole-4-carbaldehyde and N-substituted phenyl)-3-oxobutanamides/4-methyl-3-oxopentanamides and ammonia and studied for their enhancing effect on the antibacterial activities towards *S. pyogens MTCC-443, S. aureus MTCC-96* and *P. aeruginosa MTCC-441*(Gram positive) *and E. Coli MTCC-442* (Gram negative) bacterial strains and anti fungal activity towards *Aspergillus niger MTCC-282* and *A. clavatus MTCC-1323* at different concentration for their MIC values using disc diffusion method. During preliminary screening, compounds I_c,I_e,I_g,I_j showed the most enhancing effect on the antibacterial activity as compare to standard drug amoxicillin. The structures of title compounds were elucidated by the IR, NMR and Mass spectrometry and further confirmed by Elemental analyses.

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Poster Presentations

Phytochemical studies of methanolic extract of wheatgrass (*triticum aestivum*)

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ABSTRACT

Wheatgrass (*Triticum aestivum*) is the common cereal-crop that has been a staple food of man from many centuries and its juice has been used as a health tonic for several years. It is a complete protein with about 30 enzymes, 13 vitamins, several antioxidants, minerals, all 20 amino acids and contains the hormone abscisic acid (dormin), the antioxidant enzymes (viz. Superoxide Dismutase, cytochrome oxidase) and other essential nutrients. Apart from the several essential nutrients, it also contains some phytochemicals which are having medicinal values. In the present study, phytochemical analysis of methanolic extract of wheatgrass was performed on the basis of qualitative and quantitative analysis. The phytochemicals- alkaloid, flavonoid, glycosoide, carotenoid, steroid and tannin were found to be present while saponin, coumerin, terpenoid and anthraquinone were absent. In view of these above findings, the phytochemicals have been found promising biological activities.

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Photochemical bleaching of brilliant blue by sono-photo-Fenton and photo-Fenton reagent: A comparative study

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ABSTRACT

Ultrasonic irradiation is shown to accelerate the rate of photochemical bleaching of brilliant blue. This study was conducted to assess the removal efficiency of brilliant blue from aqueous medium using the photo-Fenton process in presence of ultrasonic irradiation. The Fenton's reagent consists of a mixture of H_2O_2 and Fe^{3+} was used to generate the hydroxyl radical (•OH) that attacks the target contaminant molecule and degrade it. The effect of different variables like the concentration of ferric ion, concentration of dye, pH, hydrogen peroxide, light intensity etc. on the reaction rate has been observed. The progress of the sono-photochemical degradation was monitored spectrophotometrically. The optimum sono-photochemical degradation conditions were experimentally determined. The results showed that the dye were completely oxidized and degraded into CO_2 and H_2O. A suitable tentative mechanism for sono-photochemical bleaching of brilliant blue by sono-photo-Fenton's reaction has been proposed.

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Poster Presentations

Cu-catalyzed microwave-assisted one-pot synthesis of 2-aminoimidazole-triazole framework via dimorth rearrangement and click reaction

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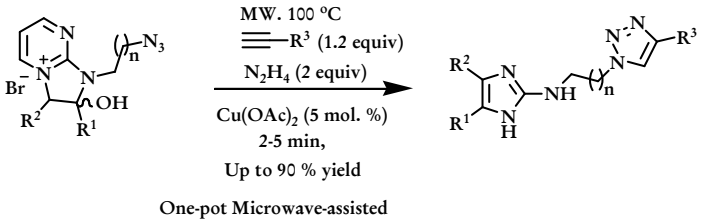
ABSTRACT

A microwave assisted one-pot Cu(II)-catalyzed protocol was developed for the construction of 2-AI-T framework. This process combining two consecutive steps of dimorth rearrangement and click reaction represents a useful protocol for the smooth synthesis of novel 2-aminoimidazole-triazole derivatives.



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Combinational effect of andrographis paniculata and silybum marianum against severe liver damage

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ABSTRACT

The effect of hydroalcoholic extract of aerial part of Andrographis paniculata, Silybum marianum and their different combination were assayed for hepatoprotective activity against CCl4 induced liver damage in rats. The extracts (100, 200 and 400 mg/kg) and their different combinations (400mg/kg) were administered orally. Liv. 52 was used as standard drug. The level of aspartate aminotransferase (AST), alanine aminotransferase (ALT) and total protein were measured. S. marianum at a dose of 400mg/kg was found to be most potent, while its combination with A. paniculata in the concentration ratio of 2:1 was found to be most effective among all tested combinations. It was concluded from the study that both the plant extracts and their combination possesses hepatoprotective activity against CCl4 induced hepatotoxicity in rats.

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Poster Presentations

Characterization of *Brugia malayi* thymidylate kinase a putative drug target

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ABSTRACT

Human lymphatic filariasis, an infectious disease caused by lymph dwelling nematode parasite, is prevalent in tropical and subtropical countries. About 1.2 billion people living in more than 83 countries worldwide are affected by this disease (WHO, 2009). In human nematode parasites *Wuchereria bancrofti*, *Brugia malayi* and *B. timori* cause this disease. Filarial worms possess both de novo and salvage pathway for purines and pyrimidines biosynthesis. Thymidylate kinase (dTMP kinase or TMK; EC 2.7.4.9) catalyses the phosphorylation of dTMP to form dTDP in both the de novo and salvage pathways of dTTP synthesis which is important precursor for DNA synthesis. *B. malayi* thymidylate kinase gene was PCR amplified from cDNA using specific primers and cloned in pGEM-T Easy cloning vector. It was further subcloned in pET-28a expression vector. Recombinant thymidylate kinase clone was transformed in C-41 cells (*E.coli* strain) for expression of protein. The protein was found to maximally expressed at 0.5 mM IPTG and 20 °C. Recombinant protein was purified by Ni-NTA affinity column and expression was confirmed by the western blotting. The kinetic studies of *Brugia malayi* thymidylate kinase showed significant differences as compared to other parasites.

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Strategy of finding novel non-peptide inhibitors of caspase-7 using phase: A novel approach to ligand based pharmacophore generation and virtual screening

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ABSTRACT

Caspase-7 belonging to a family of cysteine aspartate, also known as CASP7, is a human protein encoded by the CASP7 gene. Therapeutic inhibition of Caspase-7 has been indeed shown to prevent cells from apoptosis. In this context we have generated a chemical feature based pharmacophore hypotheses using PHASE 3.1 in the Maestro modeling environment, which exhaustively identifies spatial arrangements of functional groups that are common and essential to the biological activity of a set of high affinity ligands. 3Dpharmacophore model developed was, characterized by distinct chemical features such as Hydrogen bond acceptor, Hydrophobic, Ring aromatic that may be responsible for the activity of the Caspase-7 inhibitors. The validated 3D pharmacophore model was used to carry out a search of the Maybridge database. The results of our study provide valuable information about the novel inhibitors of Caspase-7.

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Poster Presentations

Plasmodium yoelii: Expression and purification of purine nucleotide phosphorylase

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ABSTRACT

Malaria is mosquito borne infectious disease caused by a protozoan parasite *Plasmodium*. It is widespread in tropical and subtropical regions, including parts of the Asia and Africa. Due to development of resistance against major antimalarials in malarial parasites an urgent need exists to identify new drug targets and develop new pharmacophores with unique structure and mode of action. Development of antimalarials requires understanding of host parasite interaction and characterization of biomolecules involved in metabolic system of parasite. Like other intracellular pathogens *Plasmodium* have devised mechanisms to exploit their host cells to ensure their survival and replication. The malaria parasite obtains preformed purines by the salvage pathway. It cannot synthesize purine nucleotides denovo because enzymes for denovo synthesis are absent. The primary purine salvaged by the parasite is hypoxanthine which can be obtained from the host plasma. In addition, adenosine from the host plasma can be converted to hypoxanthine by parasitic enzymes. Purine nucleoside phosphorylase (PNP) which converts inosine in to hypoxanthine, can serves as putative drug target for synthesis of new antimalarial compounds. PNP gene was PCR amplified using gene specific primers and *Plasmodium yoelii* cDNA. The cloning of the enzyme has been carried out in suitable vectors for expression of protein. Expressed protein was purified with metal –ion affinity chromatography for studying kinetic properties of parasitic enzyme.

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Poster Presentations

Artemisinin and its derivatives as inhibitors of antioxidant system of *Plasmodium yoelii*

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ABSTRACT

Malaria is amongst the most prevalent parasitic diseases in the tropics. 95% of the malarial cases are due to *P. falciparum* and *P. vivax.* The antimalarials viz., 4-aminoquinolines, 8-aminoquinolines, amino alcohols and antifolates have been used in the control and treatment of the disease, however due to increasing incidences of drug resistance in recent years development of new antimalarials is needed. Quinine resistance have been reported in *P. falciparum* from Brazil and South East Asia and Artemisinin is being used for treating such antimalarial resistance parasites. Oxidative stress is an important mechanism for the destruction of malarial and other intracellular parasites. The intra erythrocytic stages of malarial parasite encounter reactive oxygen species produced either by erythrocytes or host immune cells. In order to prevent oxidative damage, the parasite would both commandeer host enzymes and reduced its own antioxidant enzymes. The erythrocytes itself have potent antioxidant defences to counteract production of ROS by oxidation of haemoglobin of methaemoglobin. The malarial parasite contained antioxidant enzymes viz., SOD catalase and GPX in different developmental stages. The effect of Artemisinin and its derivative was studied in rodent malarial parasite *P. yoelii.* The Artemisinin and its derivative were found to inhibit the antioxidant defence enzymes of infected erythrocytes. The antimalarials affected the antioxidant enzymes of the *P. yoelii* to different extent. Incubation of Artemisinin and its derivative with infected blood for one hour also exerted significant inhibitory effect on the antioxidant system of the erythrocyte as well as parasite. Artemisinin and its derivatives appear to significantly inhibit the antioxidant system of the malarial parasite.

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Poster Presentations

L-proline in ionic liquid: An efficient and reusable catalyst for synthesis of pharmaceutically and biologically pertinent azaspiroheterocycles *via* one-pot multi-component mannich-type reaction

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ABSTRACT

Organic molecules containing a spiroheterobicyclic moiety are of broad scientific interest due to their unique chemical and conformational features as well as the biological properties often associated with the asymmetric spiro carbon atom. They have attracted considerable attention from the synthetic community. More particularly, the spiroheterobicyclic nucleus is present in a variety of natural products and biologically active compounds and can be of importance in the development of new medicinally relevant heterocyclic scaffolds. For example, a new class of marine toxins isolated from shellfish and dinoflagellate, such as pinnatoxins and pteriatoxin, exhibits an azaspiro system responsible for the biological activity. Therefore, targeting these types of heterocyclic core has long been an area of intense development and still constitutes an active domain. As a part of our ongoing research in the field of green chemistry and our continual work on the synthesis of biodynamic spiroheterocycles, we have developed a sustainable approach for the construction of highly substituted spirohexahydropyrimidines *via* a one-pot, multi-component condensation of anilines, formaldehyde, and cyclohexanones in ionic liquid using ring closure metathesis. The advantageous features of this methodology are environmentally benign character, operational simplicity with high yield processing and easier scaling up for large scale synthesis.Further, we have studied the influence of various types of ionic liquids for this transformation. The next important aspect was to examine the catalyst recovery and the possibility of reuse of the catalyst in subsequent reactions. The detailed synthetic methodology and mechanistic pathway of these compounds will be discussed in the symposium.

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Poster Presentations

PEG accelerated one pot synthesis of thiazolidinones

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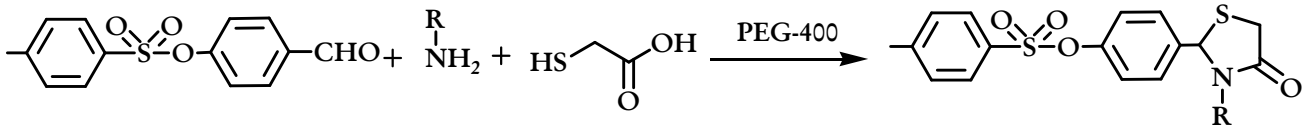
ABSTRACT

4-Thiazolidinone and its derivatives have been gaining considerable importance in the field of organic and medicinal chemistry as they display a fascinating array of pharmacological properties.[1] In view of this several synthetic routes have been developed for obtaining the heterocycles.[2] It has been noted that there is still need of safer, convenient and rapid synthetic protocol for the biodynamic 4-thiazolidinones. Keeping this in mind here attempts are made to develop a unique route for the reported and new 4-thiazolidinones using PEG- 400 as greener medium and catalyst. The route is depicted in the following scheme. The details of the synthetic route and its merits will be presented.



Scheme 1: Synthesis of 4-thiazolidinones.

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PP - 152

Poster Presentations

Surfactant catalyzed convenient and greener synthesis of tetrahydrobenzo[a]xanthene-11-ones at ambient temperatures

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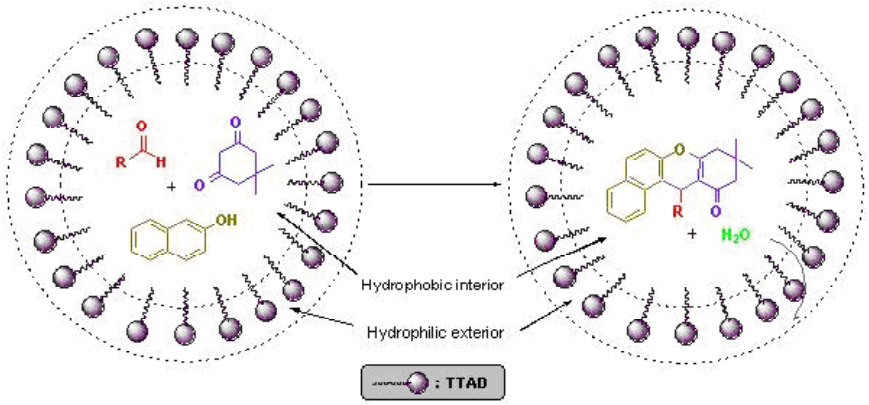
ABSTRACT

Emerging area of green chemistry demands ecofriendly organic chemical processes, considering the increasing environmental pollution and its drastic impact on living systems.[1] Hence, significance of greener pathways in organic synthesis is ever-growing in order to attain the sustainability. In this regard, water has been emerged as a safer and excellent reaction medium, since, it is not only inexpensive and environmentally benign solvent but also plays a distinguished role in reactivity and selectivity.[2] Keeping all these aspects in mind, an efficient and greener protocol for the synthesis of 12-aryl-8,9,10,12-tetrahydro-benzo[a]xanthen-11-one using tetradecyl trimethyl ammonium bromide (TTAB) at room temperature in water is described. In this method, application of TTAB has been first time introduced for performing organic transformation. Surfactant type catalyst[3] catalyzed the reaction efficiently at room temperature in short reaction times, without using any harmful organic reagents and solvents.



PP - 153

Poster Presentations

Synthesis and antimicrobial activity of some novel 6-chloro nicotinamide derivatives

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ABSTRACT

A series of new Pyrazolines,Oxazines and Thiazines having 6-Chloronicotinamide moiety have been synthesized by the condensation of 6-Chloro-{4-[(2E)-3-(Aryl) prop-2-enoyl] phenyl} pyridine-3-carboxamide with hydrazine,substituted hydrazine,urea and thiourea using appropriate catalyst and solvent respectively. The structure of the newly synthesized compounds were confirmed by analytical and IR,NMR,MASS spectral data. Antimicrobial activities of these compounds were carried out against various strains of bacteria and fungi.Some of the compounds have exhibited good activity.

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Evaluation of antimicrobial activity of swertia chirata

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ABSTRACT

Antimicrobial activity of the crude methanolic and aqueous extracts of Swertia chirata were evaluated against 10 bacteria and 3 fungi using agar diffusion method (well method). Gentamycin and Amphotericin were used as standard drug for antibacterial and antifungal activity respectively. The antimicrobial activity was determined by measuring the diameter of the zone of inhibition in term of millimeter (mm). The results showed that the methanol extract possess better significant activity than aqueous extract against of the test organisms. Both the extracts showed concentration dependent activity. The phytochemical analysis showed the presence of tannin in both the extract and flavonoids and alkaloids in methanol extract. This may be concluded that the antimicrobial activity showed by the plant due to presence of these phytochemicals.

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Poster Presentations

MW assisted facile synthesis of some chalcones and their conversion into pyrazoline derivatives containing mercaptobenzthiazole moiety: A new class of antimicrobials

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ABSTRACT

Chalcones (3a-3n) were synthesized by Claissen-Schmidt condensation involving the treatment of various substituted acetophenones with different substituted aromatic aldehydes. Pyrazoline derivatives (4a-4n) were synthesized by cyclocondensation of chalcones with hydrazides of mercaptobenzthiazole (2). The structures of the synthesized compounds have been established on the basis of IR, ^{1}H NMR and Mass spectral data. The compounds were evaluated for their antimicrobial activities.

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Poster Presentations

Synthesis of cyclohexenones as biologicaly active agents

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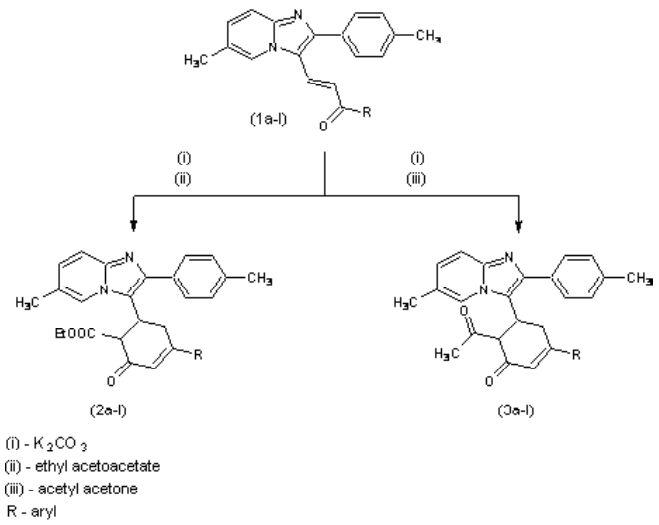
ABSTRACT

The target compounds 2a-l and 3a-l were obtained from 3-[6-methyl-2-(4-methylphenyl)imidazo[1,2-a]pyridin-3-yl]-1-(4-aryl)prop-2-en-1-one 1a–l by Michel Addition of ethyl acetoacetate and acetyl acetone in the presence of dry potassium carbonate. The structure of newly synthesized compounds has been confirmed on the basis of Elemental Analysis and (IR, ^{1}H NMR and MS) spectral studies. The pharmacological evaluation was performed for their antimicrobial activities respectively.



Scheme-1

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PP - 157

Poster Presentations

Ice chromatography: An innovative technique in separation science

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ABSTRACT

Water is one of the most eco- friendly materials, and has been utilized in a wide variety of disciplines such as synthetic chemistry, analytical chemistry, Chromatography, and many more. Water–ice is known to be involved in various natural processes. It has-been also discovered that antifreezing proteins prevent the growth of water–ice crystals in biological cells, and thereby allow organisms to live even under the freezing point of water. Thus, water–ice is an adsorbent potentially compatible as the chromatographic stationary phase, and, in addition, reactions occurring on the water–ice surface are of fundamental interest. In ice chromatography, water-ice particles are employed as a chromatographic stationary phase, has proven an efficient technique for probing the solution/ice interface. Several compounds, including estrogens, amino acids, and acyclic polyethers, have been successfully separated by ice chromatography with a hexane-based mobile phase. Water is mostly expected to replace present organic solvents that are hazardous to human health and the global environment. From this perspective, high-temperature water has been studied as the chromatographic mobile phase because water loses its specific properties that we encounter at usual temperature and shows the properties comparable to organic solvents.

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PP - 158

Poster Presentations

Novel synthesis, characterisation and activity predication of some new class of hydroxytriazenes incorporating antipyrine moiety

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ABSTRACT

Computer aided drug designing has recently attracted attention of synthetic organic chemists. PASS (Prediction of Activity Spectra for Substances) is a very simple tool for prediction probable activity theoretically on the basis of molecular structure. In the present investigation four hydroxytriazenes namely 3-hydroxy-3-(3-methyl phenyl)-1-(4,5-dimethyl-3-phenyl-3,4-dihydro-3H-pyrazol-2-one-1-yl)-triazene, 3-hydroxy-3-(4-methyl phenyl)-1-(4,5-dimethyl-3-phenyl-3,4-dihydro-3H-pyrazol-2-one-1-yl)-triazene, 3-hydroxy-3-(4-chloro phenyl)-1-(4,5-dimethyl-3-phenyl-3,4-dihydro-3H-pyrazol-2-one-1-yl)-triazene and 3-hydroxy-3-[4-(hydroxymethyl) phenyl]-1-(4,5-dimethyl-3-phenyl-3,4-dihydro-3H-pyrazol-2-one-1-yl)-triazene bearing an antipyrine moiety have been synthesized by coupling of aryl hydroxylamine obtained by reducing substituted nitrobenzenes with diazonium salt obtained from 4-amino antipyrine taking hydroxyl amine in excess at the temperature between 0-5?C. The product of coupling was washed and crystallized using appropriate solvent. Their chemical structure was confirmed by IR, ^{1}H NMR, MASS and by elemental analysis. Synthesized compounds have been screened using PASS (http://www.ibmh.msk.su/PASS) for probable activities and good antiviral, antipyretic activity along with number of other activities have been predicted. However these have to be validated by experimental bioassay. The present paper thus paves way for CADD.

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Poster Presentations

A new method for the facile synthesis of hydroxylated flavones by using allyl protection

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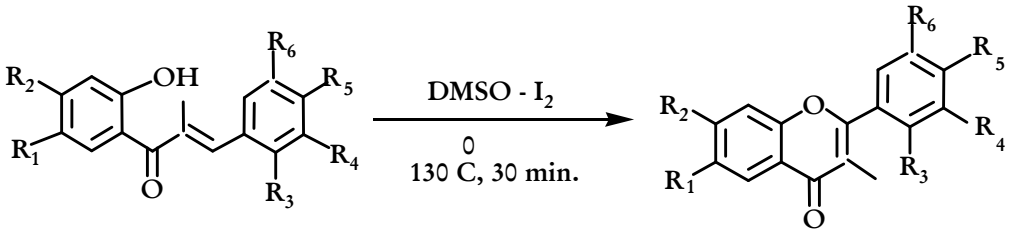
ABSTRACT

The allyl group has been frequently used in organic synthesis as a protecting group for alcohols, phenols, acids and peptides, due to its stability under basic and acidic conditions. A new method for the cleavage of allyl ethers using a catalytic amount of iodine in dimethyl sulphoxide is developed. The method is compatible with several functional groups under mild reaction conditions. Phenolic hydroxyl groups are ubiquitous in naturally occurring secondary metabolites of plants and animals. Polyphenols are oxidation prone, sensitive to radicals and possess enhanced nucleophilicity. Therefore protection of phenolic hydroxyl group in multistep synthesis of biologically important natural product flavonoids; including chalcones, flavanones and flavones is immense important. In the natural product flavone invariably OH or OMe groups are present as one of the substituents. We were interested in the protection of phenolic group in phenols, aldehydes and ketones which were used in the synthesis of chalcones. The allyl protected hydroxy chalcones are oxidatively cyclised to flavones by using a catalytic amount of iodine in dimethyl sulphoxide.



R_3 = O-allyl
R_1, R_2, R_4, R_5, R_6 = Cl, Br, alkyl, alkoxy

R_3 = OH
R_1, R_2, R_4, R_5, R_6 = Cl, Br, alkyl, alkoxy

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Poster Presentations

Synthesis, characterization and antimicrobial activity of some new quinoline-oxadiazole-azetidinone derivatives

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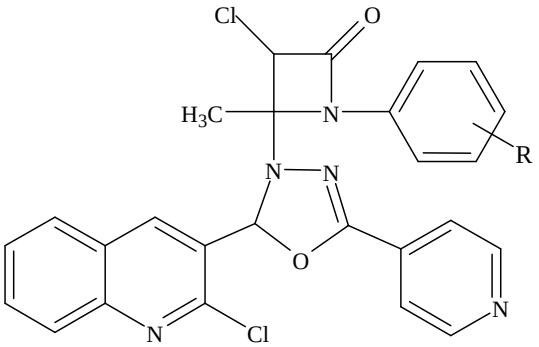
ABSTRACT

The quinoline nucleus is an important class of heterocyclic compound found in many synthetic and natural products with a wide range of pharmacological activities, such as antimalarial,[1] anti-inflammatory,[2] antiasthmatic,[3] antibacterial[4] and tyrosine kinase inhibiting agents.[5] The chemistry of 1,3,4-oxadiazoles have received considerable attention from synthetic organic chemists due to their diverse biological activities.[6-8] Several research groups have contributed to the development of methods for the synthesis of 1,3,4-oxadiazoles.[9-11], The β-lactam drugs are most widely prescribed as antibiotics and used in therapeutics. Azetidinone and its derivatives are also very good antibacterial,[12] antitubercular,[13] and antifungal[14] agents and possess pharmacological properties.[15] However, these procedures are time consuming and proceed in low yields. Therefore, a convenient and eco-friendly method for the synthesis of 1,3,4-oxadiazoles is highly desirable. Looking to the medicinal importance, we have synthesized 3-chloro-4-[2-(2- chloro(3-quinolyl))-5-(4-pyridyl)(1,3,4-oxadiazolin-3-yl)]-1-(aryl)4-methylazetidin-2-ones. Structural elucidation of the newly synthesized compounds was done by elemental analysis, IR, ^{1}H-NMR spectra, ^{13}C-NMR and mass spectra. The purity of all the compounds has been checked by thin layer chromatography. All the final compounds have been evaluated for their *in vitro* antibacterial activity and antifungal activity against different strains of bacteria and fungi.



R = Different substituents

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Poster Presentations

Synthesis of 2-oxo-azetidine derivatives as potential antimicrobial agents

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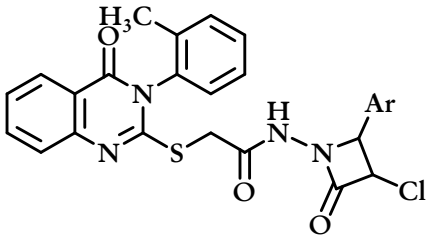
ABSTRACT

A series of N-[2-(aryl)-3-chloro-4-oxo-azetidine-1-yl]-2-(6-bromo-4-oxo-3-o-tolyl -3,4-dihydro-quinazolin-2-ylsulfanyl)-acetamides have been synthesized, characterized and screened for antimicrobial activity. A mixture of carbon disulfide and o-toludine was added drop wise to a refluxing mixture of 2-amino-5-bromo-benzoic acid and potassium hydroxide in methanol. The mixture was heated under reflux for 12 hrs, to get the product, dissolved in10% potassium hydroxide and con. HCl is added and filtrated. The solid product is obtained. The eqimolar solution of compound 1 and ethyl chloro acetate in dry acetone in presence of K_2CO_3, was refluxed on a water bath for about 42 hrs. The reaction mixture was poured in ice to get a solid product compound 2. The compound 2 and hydrazine hydrate were added in methanol the refluxing time is 4 hrs, during the refluxing, acetic acid(2-3drops) was added in this situation, solid product obtained, filtered and wash with water to get compound 3. Compound 3 and different aryl aldehydes in methanol was refluxed for 8 hrs and filtered then wash with water to get compound 4a-l. Compound 4a-l in dioxane was taken in a flat bottom flask and stirred at 5-10°C. During the stirring triethyl amine and chloro acetyl chloride were added and stirred another half an hour. And then reaction mixture was refluxed for 5hrs. Filtered the reaction mixture for removal of triethylamine hydrochloride and poured the filtrate in ice cold water to get a precipitate of compound 5a-l. Series of synthesized compounds 5a-l were screened for their antimicrobial activity against different types of bacteria and fungus.



(Where Ar = different aryl group)

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Poster Presentations

Studies on synthesis, characterization and antimicrobial evaluation of some medicinally important 1, 3, 4-oxadiazoles

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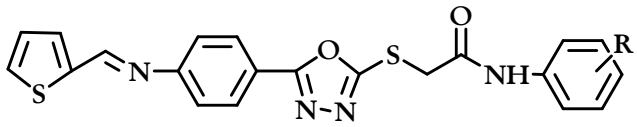
ABSTRACT

1, 3, 4-Oxadiazole is a thermally stable aromatic heterocycle and is of chemical and biological interest since long due to their interesting therapeutic activities like antifungal,[1] anti-inflammatory,[2] analgesic,[3] anticonvulsant,[4] antihypoglycemic[5] and antibacterial[6] activities. They also possessed anti-cancer activity[7] and also act as muscle relaxants.[8] In continuation to this , we have prepared 5-{4-[1-aza-2-(2-thienyl)vinyl]phenyl}-1,3,4-oxadiazole-2-thiol as an intermediate compound for the synthesis of some new 2-{5-[4-(1-aza-2-(2-thienyl)vinyl)phenyl](1,3,4-oxadiazol-2-ylthio)}-*N*-(aryl)acetamides. The purity of the compounds was proved by thin layer chromatography and the structures of these compounds were elucidated by using IR, ^{1}H NMR and mass spectroscopy. The newly synthesized compounds have been screened for biological screening on several strains of bacteria and fungi.



Where R = Different substituents

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Poster Presentations

Synthesis and biological screening of some new 1,3,4-oxadiazole derivatives

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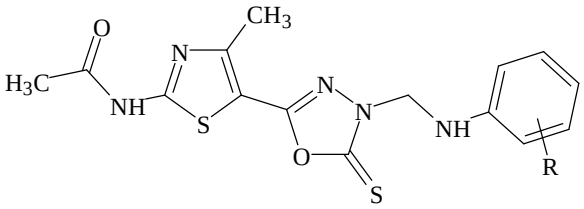
ABSTRACT

Looking to the medicinal importance of thiazole and 1,3,4-oxadiazole, we have decided the incorporation of both the moieties in one frame work to explore the synthesis of more potential bioactive molecules. The thiazole ring has been extensively studied and it is present in several heterocyclic moieties like Thiamine[1] (Vitamin B_1), Penicillins and antibacterial thiazoles.[2] Moreover, a number of thiazole derivatives exhibit pharmacological activities like anti-inflammatory, anthelmintic, fungicidal etc.1,3,4-oxadiazole derivatives have been reported to be biologically versatile compounds having hypnotic, analgesic[3] and anti-inflammatory,[4] vasodilator, antitussive and anticancer[5] activities. The preparation of novel *N*-[5-(3-{[(aryl)amino]methyl}-2-thioxo (1,3,4-oxadiazolin-5-yl))-4-methyl-1,3-thiazol-2-yl]acetamides were carried out by the condensation of substituted thiazolyl hydrazide with carbon disulphide in presence of base to furnish 1,3,4-oxadiazole nucleus[3,6] followed by Mannich reaction to produce Mannich base. The synthesized compounds were characterized by FT-IR, ^{1}H NMR and mass spectra. The biological activity of these compounds was carried out on several strains of bacteria and fungi.



R= Different substituents

PP - 164

Poster Presentations

Synthesis and antibacterial activity of some pyridine derivatives containing benzimidazole and thiazolidine moieties

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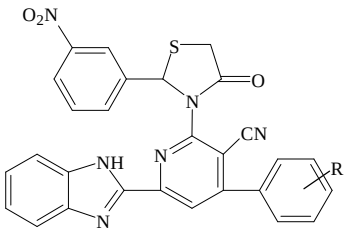
ABSTRACT

Pyridine derivatives have attracted more interest in recent years because of their various biological and pharmacological activities and have raised considerable interest because of their potential beneficial effects on human health.[1,2] It was found that when one biodynamic heterocyclic system was coupled with another heterocyclic system, enhanced biological activity was produced. Looking to the literature survey and pharmacological importance of pyridine,[3] benzimidazole[4] and thiazolidine,[5] we have coupled three moieties in one heterocyclic moiety and tried to synthesize a series of 6-benzimidazol-2-yl-4-(aryl)-2-[2-(3-nitrophenyl)-4-oxo(1,3-thiazolidin-3-yl)]pyridine-3-carbonitriles. The compounds were characterized by FT-IR, ^{1}H NMR, mass spectroscopy and elemental analysis. All the newly synthesized compounds were evaluated for their antibacterial and antifungal activities against several strains of bacteria and fungi.



R = Different substituents

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Poster Presentations

Facile synthesis of a series of quinoline based 2-pyridone and thiazole heterocycles involving Vilsmeier-Haack synthesis and Hantzsch's synthesis

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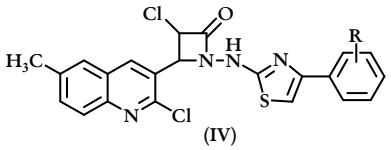
ABSTRACT

Looking to the biological importance of quinoline,[1-4] thiazole[5-7] and azetidinones,[8-11] we have incorporated all the three heterocycles in a single frame work. Vilsmeier-Haack[12] synthesis was used to prepare 2-chloro-6-methylquinoline-3-carbaldehyde (I), which on further treatment with thiosemicarbazide gave the schiff base 2-((2-chloro-6-methylquinolin-3-yl)methylene)hydrazine- carbothioamide (II). Compound (II) on cyclization by Hantzsch's synthesis with different α-halogenoketones gave 2-(2-((2-chloro-6-methylquinolin-3-yl)methylene)hydrazinyl)-4-arylthiazoles (III), which when treated with chloroacetyl chloride in presence of triethylamine furnished series of azetidinone containing 3-chloro-4-(2-chloro-6-methylquinolin-3-yl)-1-(4-arylthiazol-2-ylamino) azetidin-2-ones (IV). All the newly synthesized compounds were characterized by IR, NMR and mass spectra and screened for their antibacterial and antifungal activities.



(IV)

R = Different substituents

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Poster Presentations

Isolation and characterization of anthraquinone derivatives from *Cassia fistula* using chromatographic and spectral techniques

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ABSTRACT

Present study involves characteristic evaluation of medicinally important ingredients like anthraquinone derivatives from *cassia* family. *Cassia* family is well-known source of anthraquinone glycosides and their derivatives in the various parts of plants. We have selected *cassia fistula* plant from *cassia family* in the present study because it contains anthraquinone derivatives in sufficient concentration. The present work was carried out to separate and characterize three major ingredients of anthraquinone derivatives such as 1,3,8-Trihydroxy-6-methyl-anthraquinone (emodin), 4,5-Dihydroxy-9,10-dioxo-4a,9,9a,10-tetrahydro-anthracene-2-carboxylic acid (rhein) and 1,8-Dihydroxy-3-methyl-anthraquinone (chrysophenic-acid). These three constituents were found in predominant concentration and therefore, we have isolated as a single component by using chromatographic techniques and their characterization was done by different spectral methods like NMR and Mass spectroscopy. The crude extract of *cassia fistula* was used for the treatment of various skin disordered. The 0.1% to 0.5% concentration of crude was prepared in the petroleum jelly (inert base) and patients attending O.P.D. at Tapibai Ayurvedic Hospital of Bhavnagar were selected randomly (irrespective of their age, sex, marital status, religion), suffering from skin disorders and categorized from the apparent dermatological symptoms under the supervision of qualified doctor. The results were found encouraging and patients suffering from ringworm were cured completely within four week of first applied on the effected part of skin and out of 52 patients 48% of the patients have been cured completely.

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Poster Presentations

Synthesis and antimicrobial evaluation of medicinally important imidazole derivatives

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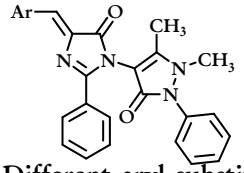
ABSTRACT

Imidazole is a vital heterocyclic nucleus, which is well known for its wide biological profile[1]. Imidazole derivatives have been associated with a wide array of pharmacological activities including antimicrobial,[2,3] anti-inflammatory[4] and analgesic,[5,6] antitubercular,[7] cytotoxic,[8] antiviral[9] and antimuscarinic.[10] The pharmacological importance of imidazole prompted us for further modification of heterocyclic framework to synthesize some new 5-oxo-imidazole derivatives. In the present work, we have used 4-amino-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one as an intermediate compound for the synthesis of some novel 4-(4-arylidene-5-oxo-2-phenyl-4,5-dihydro-1*H*-imidazol-1-yl)-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-ones. Structural elucidation of the newly synthesized compounds was done by elemental analysis, IR, ^{1}H NMR and mass spectral data. The purity of all the compounds have been checked by thin layer chromatography. All the products have been evaluated for their growth inhibitory activity against different microbes in order to study their pharmacological profile.



Ar = Different aryl substituents

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Poster Presentations

Synthesis and antimicrobial activity of novel benzimidazole containing 2-oxopyridine derivatives

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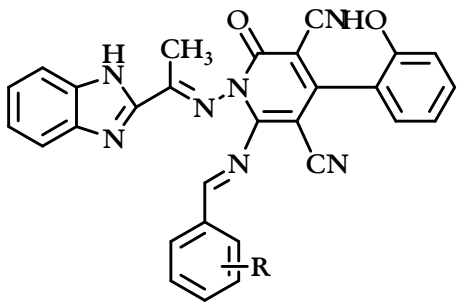
ABSTRACT

Benzimidazole and 2-oxopyridine are vital heterocyclic nuclei which are well known for their wide biological profile. Benzimidazole ring is an important pharmacophore in modern drug discovery.[1] Benzimidazole derivatives exhibit significant activity against several viruses and bacteria such as HIV,[2] RNA,[3] herpes (HSV-1),[4] influenza,[5] human cytomegalovirus (HCMV),[2a] antifungal,[6] anthelmintic,[7] antihistaminic,[8] antiulcer,[9] cardiotonic,[10] and neuroleptic.[11] 2-Oxopyridine is also found to possess useful pharmacological activities such as analgesic, antifungal, antimalarial, anti-inflammatory, antibacterial, anti-HIV, phytotoxic, antitumor, and antiviral.[12-20] In addition, benzimidazole and 2-oxopyridine derivatives have played a crucial role in the theoretical development of heterocyclic chemistry and are also used extensively in organic synthesis. This inspired us to combine these two moieties in one frame for further enhancing their pharmacological activities. A series of 1-(1-(1*H*-benzimidazole-2-yl)ethylideneamino)-6-(arylideneamino)-4-(2-hydroxyphenyl)-2-oxo-1,2-dihydropyridine-3,5-dicarbonitriles have been synthesized. The purity of all the compounds has been checked by thin layer chromatography. Structural elucidation of the newly synthesized compounds was done by elemental analysis, IR spectra, ^{1}H NMR and ^{13}C NMR and mass spectra. All the bioactive molecules have been evaluated for *in vitro* antibacterial activity against *E. Coli, P. aeruginosa, S.aureus and S.pyogenus* and screened for antifungal activity against *C. albicans, A. niger and A. Clavatus.*



R= Different substituents

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Poster Presentations

Synthesis and antimicrobial screening of some new [1,2,4]-triazole-3-thione derivatives

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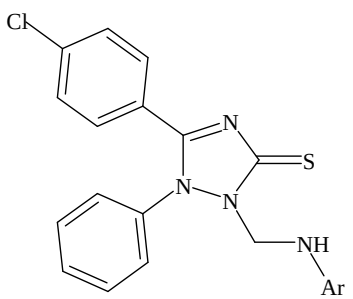
ABSTRACT

Mannich bases are associated with a wide variety of biological activities and industrial applications such as, antiinflammatory,[1-3] anticancer,[4] tranquilizing,[5-6] Analgesic,[7] Antifungal,[8] Antibacterial,[9] Antipsychotic,[10] Antitumor,[11] Antileishmanial[12] and Antimalarial.[13-17] 4-Chloro benzoyl isothiocyanate 1 was prepared by a reaction of 4-chloro benzoyl chloride and ammonium isothiocyanate in dry acetone with constant stirring at room temperature. Compound 1 reacts with phenyl hydrazine in the presence of dry acetone to form 5-(4-chloro phenyl)-1-phenyl-1,2-dihydro-[1,2,4]triazole-3-thione 2. Compounds 2 on reaction with formaldehyde and different aromatic amines in 1,4-dioxane yielded 5-(4-chloro-phenyl)-1-phenyl-2-phenylaminomethyl-1,2-dihydro-[1,2,4]triazole-3-thione 3a-j respectively. The synthesized compound 3a-j was screened for their antibacterial & antifungal activities. On the basis of the results of antibacterial activity, it has been observed that compounds, 3f and 3h were found moderately active. The results 200 & 250 μg/ml are considered as a good active and 100 μg/ml is considered as an excellent active. Compounds 3c, 3f, 3h and 3j were found good active. There is no a single compound as potential as compared to standard drug against *A. niger*. 3b and 3f were found good active against *A. clavatus*. The synthesized compounds were characterized by spectral techniques like FT-IR, ^{1}H NMR & Mass spectroscopy.



Where, Ar = Different aryl groups

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Poster Presentations

Liquid-phase catalytic hydroxylation of phenol using Fe(III) complexes encapsulated in zeolite-y as catalysts for pharmaceutically active ingredients

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ABSTRACT

Encapsulation of metal complexes acting as homogeneous catalysts in the super cages of zeolite-Y matrix provides an ideal solution for the heterogenization. We have synthesized Fe(III) complexes of various Schiff bases such as vanillin-thiophene-2-carboxylic hydrazide (VTCH), ethylvanillin-thiophene-2-carboxylic hydrazide (EVTCH), vanillin-furoic-2-carboxylic hydrazide (VFCH), ethylvanillin-furoic-2-carboxylic hydrazide (EVFCH), salicylaldehyde-thiophene-2-carboxylic hydrazide (STCH) and salicylaldehyde-furoic-2-carboxylic hydrazide (SFCH) encapsulated in the super cages of zeolite-Y and characterized by various physico-chemical techniques such as ICP-OES, elemental analyses, magnetic measurements, (FTIR and electronic) spectral studies, BET, scanning electron micrographs (SEMs) as well as X-ray diffraction patterns. These encapsulated complexes catalyze the liquid-phase hydroxylation of phenol with H_2O_2 to catechol as a major product and hydroquinone as a minor product. Considering the concentration of substrate and oxidant, amount of catalyst, temperature of the reaction and volume of solvent, a best-suited reaction condition has been optimized to get maximum hydroxylation. Under the optimized reaction conditions, Fe(III)YSTCH has shown the highest conversion of 39.2% after 6 h. All these catalysts are more selective towards catechol formation (~85%), irrespective of their catalytic performance. These compounds are in a great demand for the manufacturing of pharmaceutically active ingredients.

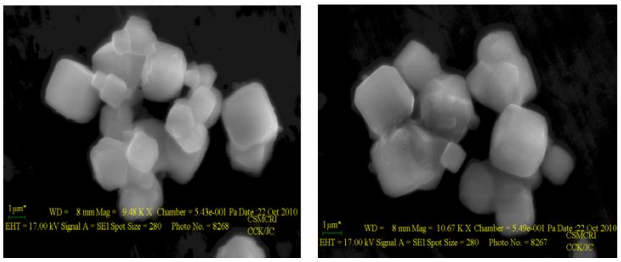

Figure 1: SEM images of Fe(III)YSTCH and Fe(III)YVTCH compounds

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Poster Presentations

Separation and characterization of phytochemicals from *Butea monosperma*

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ABSTRACT

The genus *Butea monosperma* is well known medicinal plant. It is well documented that *Butea monosperma* species contents have many medicinal efficacies, including cercaricidal property, molluscicidal activity, potent inhibitory action, antimicrobial activity, *in-vitro* pediculicidal activity, anti-inflammatory and analgesic effects. These phenolics were separated and identified using prep-HPLC-PDA technique. The standard addition method was used for method validation process and calibration curves were prepared using list-square fit method. Among the separated eight components, five were identified and characterized by using GC-MS technique. The names of five phenolics, which were separated and characterized are 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4*H*-chromen-4-one, 3,4,5-trihydroxybenzoic acid, 4-allyl-2-methoxyphenol, 2-(4-hydroxy-3-(3,4,5-tri hydroxyl-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yloxy)phenyl)-7-(3,4,5-trihydroxy-6 hydroxy methyl) tetrahydro-2H-pyran-2-yloxy)chroman-4-one (Iso-butrin) and (E)-3-(4-hydroxy-3-(3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yloxy)phenyl)-1-(2-hydroxy-4-(3,4,5-trihydroxy-6 hydroxymethyl)tetrahydro-2H-pyran-2-yloxy)phenyl) prop-2-en-1-one (Butrin).

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Poster Presentations

Characterization of some antioxidants from minor millets like *Eleusine coracana* and *Paspalum scorbiculatum* using prep-HPLC-PDA: Contribution to overall antioxidant effect

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ABSTRACT

Eleasine Corcana and *Paspalum scorbiculatum* are important minor millets of the population in the Indian subcontinent for phenolics contents. These phenolics were separated and identified by using prep-HPLC-PDA technique. The standard addition method was used for method validation process and calibration curves were prepared using list-square fit method. Among the separated twelve ingredients, eight were identified and well characterized by using GC-MS technique. The names of eight phenolics, which were separated and characterized are 3,4,5-trihydroxy benzoic acid, 3-(3,4-dihydroxyphenyl)acrylic acid, 4-hydroxy-3-methoxybenzoic acid, 3-phenylprop-2-enoic acid, 3-(4-hydroxy-3-methoxyphenyl)acrylic acid, 2-hydroxybenzoic acid, 4-hydroxybenzoic acid and 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chrmen-4-one. The identified components were also quantified and their antioxidant activities were evaluated based on rancidity of sunflower oil using in the presence of blank media like MeOH.

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Poster Presentations

Synthesis, biological studies and spectral characterization of some novel pyrazole derivatives containing benzimidazole as a coupling moiety

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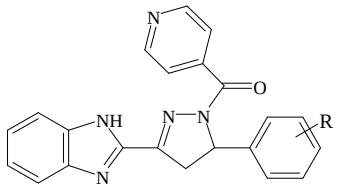
ABSTRACT

Pyrazoles are novel class of heterocyclic compounds possessing wide variety of applications in Medicinal Chemistry.[1] Derivatives of pyrazoles are found to possess antibacterial,[2] anti-inflammatory,[3] analgesic,[4] anticancer,[5] anti-convulsant[6] and anti-depressant[7] activities. Recently benzimidazoles have been studied extensively due to biological activities such as, antihistaminic,[8] antiulcer,[9] cardiotonic[10] and antihypertensive.[11] Looking to the pharmacological importance of both scaffolds, a series of 3-benzimidazol-2-yl-5-(aryl)(2-pyrazolinyl)-4-pyridyl ketones have been synthesized and characterized by FT-IR, ^{1}H NMR, Mass spectroscopy and elemental analysis. All the newly synthesized compounds were evaluated for their antibacterial and antifungal activities.



R = Different substituents

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Poster Presentations

Polymer supported mitsunobu reaction for convenient synthesis of fluoxetine scaffold

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ABSTRACT

Fluoxetine is a widely used antidepressant drug which works as selective serotonin reuptake inhibitor. Despite its high efficacy, it has several side effects especially it induces liver and renal impairment, accumulation in brain, anorexia and suicidal tendency. In view of its unacceptable side effects, we desired to synthesize various molecules based on fluoxetine scaffold in hope to further optimize its selective serotonin reuptake inhibitor activity. In developing efficient chemistry towards Fluoxetine scaffold we developed an environmentally benign route for third step in its synthesis. In this step, to couple various phenols, we optimized the use of polymer supported triphenylphosphine, which circumvented the problem triphenylphosphine oxide (TPPO) contaminating the environment and final product.

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Cloning of glucose-6-phosphate dehydrogenase of *brugia malayi*

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ABSTRACT

Filariasis (elephantiasis) caused by *Wuchereria bancrofti* and *Brugia malayi* is endemic in tropical and subtropical countries and annually affects about 120 million people worldwide. The filarial parasites mainly depend upon carbohydrate for their energy requirements. Pentose phosphate pathway (PPP) is an important metabolic pathway for yielding reducing power in the form of NADPH and pentose sugar needed for nucleic acid synthesis. Glucose-6-phosphate dehydrogenase (G6PD) is the first enzyme of the pentose phosphate pathway that converts a-D-glucose-6-phospate into D-glucono-1,5-lactone-6-phosphate. The cloning of Brugia malayi G6PD was carried out by isolating RNA from the parasite and synthesis of cDNA. G6PD gene was PCR amplified from cDNA using specific primers and was cloned in pGEM®-T Easy cloning vector. The positive clones were confirmed by restriction digestion and sequencing of the clones. These clones were sub cloned in the pTriEx-4 expression vector. Recombinant G6PD clone was transformed in *E. coli* C-41 cells for expression of protein. Recombinant protein was purified by Ni-NTA affinity column and expression was confirmed by the western blotting. The native BmG6PD is a tetramer with subunit molecular weight of 69kDa. CD analysis indicated that BmG6PD is composed of 37% a-helices and 26% ß-sheets. Kinetic properties of the purified protein showed significant differences as compared to enzyme from other parasites.

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Poster Presentations

Phytochemical characterisation of *Taverniera cuneifolia* Arn. – A potential substitute of *Glycyrrhiza glabra* L.

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ABSTRACT

Taverniera cuneifolia (Roth) Arn., often referred as Indian liquorice belonging to the family of Fabaceae (Papilionaceae) is known for a sweet component from the roots which is similar to that of *Glycyrrhiza glabra* L., popularly known as commercial liquorice. The roots of *G. glabra* are very widely used in traditional systems of medicines all over the world[1]. *G. glabra* is rich in bioactivities like antiviral, anticancer, anti-ulcer, anti-diabetic, anti-inflammatory, anti-oxidant, anti-thrombic, anti-malarial, anti-fungal, anti-bacterial, estrogenic, immuno-stimulant, anti-allergenic and expectorant, promoting expectoration, an agent that promotes expectoration activities[2-6]. The commercial liquorice has a huge demand in the Indian system of medicine, and is a major requirement of the Ayurvedic drug industry in India. This requirement is met through import from Afghanistan and Pakistan[ix]. A number of plants are often referred as Indian liquorices[3] however, a potential indigenous alternative to *G. glabra* is not yet available. *Taverniera cuneifolia* could be a potential substitute of *G. glabra* owing to the presence of a glycoside (8-13%) which is similar to glycyrrhizin.

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Poster Presentations

Novel nitroreductive prodrugs of 5-aminosalicylic acid for colon targeted drug release: Synthesis, molecular docking and kinetic studies

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ABSTRACT

Novel nitroreductive prodrugs of 5-aminosalicylic acid (5-ASA) were designed for colon specific drug release. 2-hydroxy-5-[[(Z)-2-methyl-3-(nitrophenyl)prop-2'-enoyl] amino]benzoic acid derivatives were synthesized from different nitrocinnamaldhyde, with 5-ASA and from different nitrocinnamic acid with 5-ASA. Nitroreductive prodrugs of 5-aminosalicylic acid were evaluated for inflammatory bowel disease (IBD), Chronic IBD which may be divided into two major groups, ulcerative colitis (UC) and *Crohn's* disease (CD), clinically characterized by recurrent inflammatory involvement of intestinal segments. Quantitative estimation for release profile of 5-aminosalicylic acid and *In-vitro* kinetic studies were performed by UV, HPTLC method. Nitroreductase activity was perfomed by nitroreductase *Escherichia coli* B (NTR) enzyme, extracted from rat fecal matters and the cumulated release profile of 5-ASA from synthesized prodrugs after 5 hr. was found to be 60 and 68%. 4- Nitro substituted cinnamic acid derivatives were better for the prodrug designing. Additional molecular docking was performed using AUTO DOCK 4.2 and result revealed that 3-nitro substituted analogs are poor candidates against nitroreductase *Escherichia coli* B (NTR) enzyme, but 4-nitro substituted analogs are good candidates for nitroreductase enzyme. Result of Kinetic release indicates that amide linkage in between nitrocinnamic acid and 5-ASA is a better for designing the prodrug to release 5-ASA in presence of colon specific nitroreductase enzyme.

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Poster Presentations

Synthesis and antifungal activity of some functionalized pyrimidines

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ABSTRACT

The study on antifungal chemotherapy revealed that the wide spread use of common antifungal agents (polyenes, azoles and allylamines, griseofulvin and 5-fluorocytosine) has resulted in the development of the resistance to these drugs by pathogenic microorganisms, causing an increase in morbidity and mortality, therefore new therapeutics options are required. In view of the above mentioned facts and in the continuation of our work to synthesize the novel pyrimidine of biological significant, herein, we have synthesized the various functionalized pyrimidine derivatives, 6-(3-pyridyl)-2-substitutedthio-4-oxo-3H-pyrimidine-5-carbonitriles and 2-sustitutedthio-4-chloro-6-(3-pyridyl)pyrimidine-5-carbonitriles and the synthesized compounds were subjected for their in vitro antifungal screening using to fold serial dilution assay[1-3] against the human pathogenic fungi.. Some of the synthesized compounds have displayed promising antifungal activity. In this paper the synthesis, isolation, characterizations (^{1}H NMR, Mass and IR,) and detailed antifungal activity of the synthesized compounds will be presented.

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Poster Presentations

Synthesis and biological screening of some novel 2-heteryl chromones

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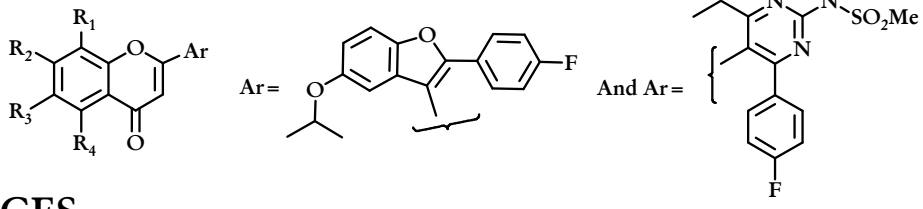
ABSTRACT

Molecules with heteroatoms rings are widely distributed in nature. Indeed a number of heterocyclic compounds like chromones, benzofurans, pyrimidines exhibit a variety of important biological activities. The chemistry of chromones and its derivatives has been studied for over a century or more, due to their diverse biological activities. Biological activities associated with this nucleus are antibacterial, antifungal, anticholesterenic, antidiabetics, antiallergic diuretics etc. Chromones having heterocyclic substituents at 2-position and 3-position have been reported to possess coronary-dilatory activity, muscular relaxation effect and antimicrobial activities. The chemistry of pyrimidines and its derivatives has been studied for their diverse biological activities like antibacterial, antiviral, antitumor, antihypertensive and antiinflamatory activities. Benzofurans are associated with biological activities like antifungal, antibacterial, anti-inflammatory and antiallergic. Therefore it was thought worthwhile to prepare some novel derivatives chromones having pyrimidine and benzofuran moiety at 2-position.



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Poster Presentations

Synthesis of novel fluorinated pyrazolyl analogues of chalcones and their derivatives as a potential antibacterial and antioxidant agents

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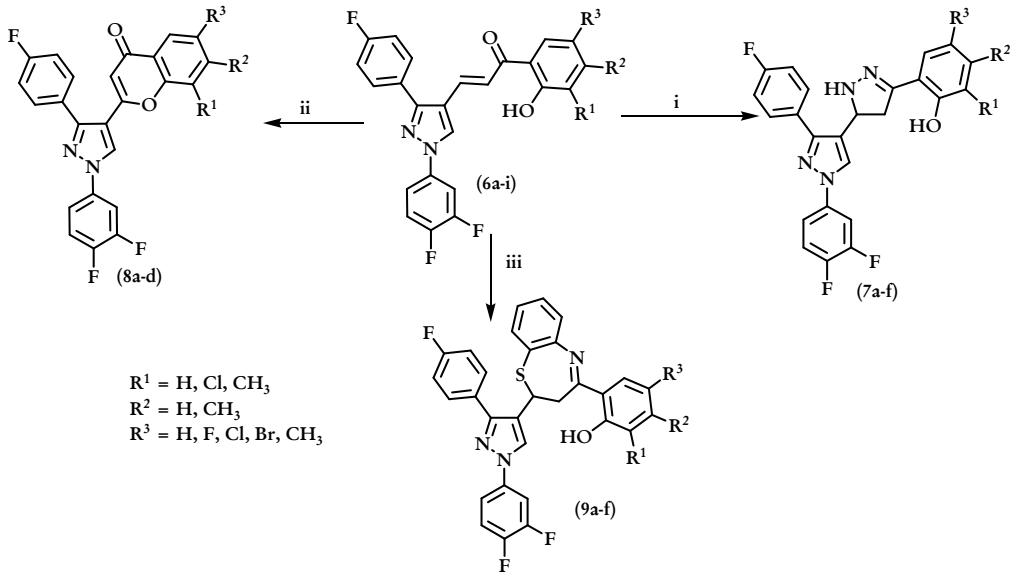
ABSTRACT

A new series of 3-(1-(3, 4-difluorophenyl)-3-(4-fluorophenyl)-1*H*-pyrazol-4-yl)-1-(2-hydroxyaryl) prop-2-en-1-one analogues (6a-i) were synthesized through Claisen-Schmidt reaction. Pyrazolyl chalcones (6a-i) on different cyclocondensation reactions afforded the racemic 2-(5-(1-(3,4-difluorophenyl)-3-(4-fluorophenyl)-1*H*-pyrazol-4-yl)-4,5-dihydro-1*H*-pyrazol-3-yl) phenol derivatives (7a-f), 2-(1-(3,4-difluorophenyl)-3-(4-fluorophenyl)-1*H*-pyrazol-4-yl)-4*H*-substituted-chromen-4-one derivatives (8a-d) and 2-(2-(1-(3,4-difluorophenyl)-3-(4-fluorophenyl)-1*H*-pyrazol-4-yl)-2,3dihydrobenzo[*b*][1,4] thiazepin-4-yl) phenol derivatives (9a-f). All the newly synthesized compounds were investigated for antibacterial and antioxidant activities.



Scheme 1

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Poster Presentations

Heteroaryl hydroxycarbonylation: An efficient, robust, practically scalable approach using formyl acetate as the co source

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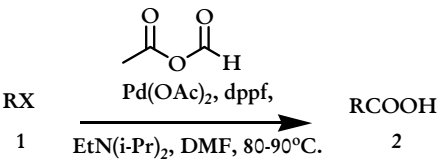
ABSTRACT

The functionalization of organic molecules with carbon monoxide as a carbonyl source has become an important and convenient method for the selective preparation of intermediates of naturally or biologically active products, pharmaceuticals and fine chemicals. Thus, a broad range of high-valuable compounds such as aldehyde, ketones, carboxylic acid derivatives, lactones, etc., are accessible from organic halides or unsaturated substrates in one step. Although much research effort has been done in this field, there still exists considerable interest in the exploration of facile and innovative synthetic strategies. From an industrial point of view, the carbonylation of hetero aryl halides, is of special interest since the resulting products (carboxylic acid and their derivatives) are valuable intermediates for the synthesis of biologically active compounds such as herbicides or pharmaceuticals. Beside methodological improvements, intermolecular carbonylation reactions of aryl, hetero aryl halides and triflates have been applied in numerous syntheses of biologically active heterocyclic compounds and natural products. Although, the carbonylation using carbon monoxide has been widely developed in past decades, it suffers from some major disadvantages like difficulty in handling toxic, gaseous carbon monoxide along with its storage and transport in chemical industries represents an authentic problems. To overcome the direct usage of carbon monoxide, the development of in situ generation of carbon monoxide is a valid target of great interest to synthetic organic chemists. We disclose herein, an operationally simple, efficient, regioselective and industrially feasible safe Hydroxycarbonylation in heterocyclic halogenated compounds using acetic-formic anhydride (stable liquid source of carbon monoxide) and Pd $(OAc)_2$ as a metal catalyst, dppf ligand and EtN $(i\text{-}Pr)_2$ as a base (Scheme 1).



Scheme 1: General scheme for heteroaryl hydroxycarbonylation

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Poster Presentations

Synthesis and biological evaluation of novel N-aroyl hydrazones and N-acylhydrazones of substituted 1-indanone - A potential antitubercular agents

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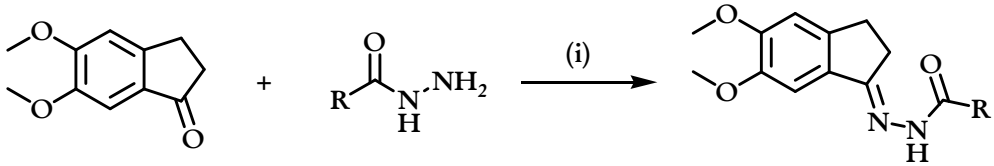
ABSTRACT

Hydrazones are organic compounds characterized by the presence of –NH–N=C< group in their molecule. N-Acyl and N- Aroyl Hydrazones have an additional donor site like >C=O, which determine the versatility and flexibility of these compounds. Such molecules and their complexes _ENREF_1[1] have been demonstrated to possess: anti- convulsant, anti- depressant, analgesic, antimicrobial, antitumor, anti-platelet, vasodilator, antiviral activity and other [2]. 1-indanones are intermediates for the synthesis of a wide variety of heterocyclic ring systems, pharmaceutical substances, natural products and other ingredients. N-aroyl and N-acylhydrazones (I) were synthesized by the condensation of 5, 6-dimethoxy-1-indanone and substituted hydrazones. The constitution of the products has been supported by elemental analysis, IR. ,^{1H}NMR , and Mass spectral data. The products have been screened for their (a) in vitro growth inhibitory activity against several microorganisms and (b) in vivo anti- tuberculosis activity.



(i) Conc. HCl, EtOH Reflux 2-6 hrs.[3]

(I) R= Aryl or Alkyl

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Poster Presentations

H_2SO_4 promoted regioselective and stereoselective synthesis of (*E*)-stilbenes from substituted phenylacetones and substituted benzaldehydes

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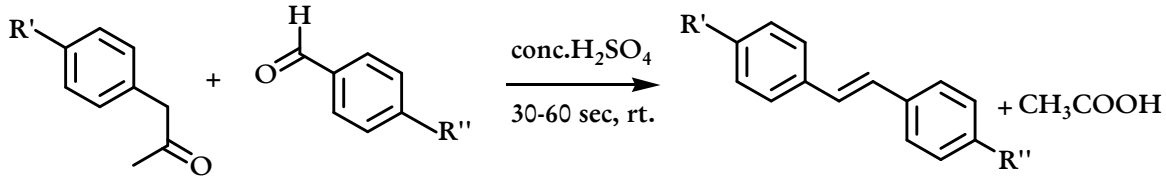
ABSTRACT

An efficient, simple and practical method has been developed to regeoselectively and stereoselectively synthesize (E)-stilbenes using H_2SO_4 as a catalyst in a short duration of time (30-60 sec.) at room temperature in good to excellent yields.



R' = H, Cl, OMe; R'' = H, Me, OH, *i*pr, OMe, OAc, Cl etc.

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Poster Presentations

Isolation, characterization, chemical transformation of alkaloidal amides of *Aegle marmelos* and study of their antifungal activity

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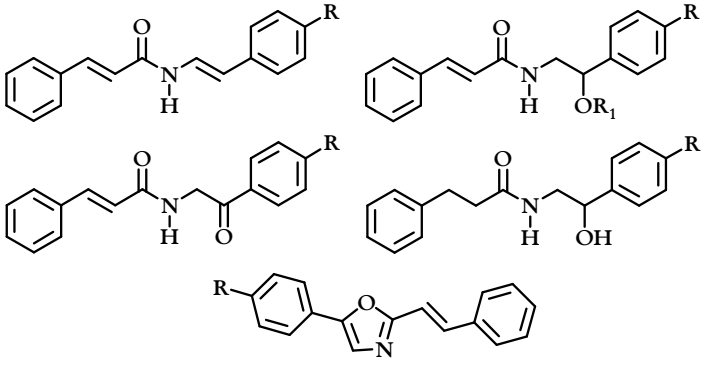
ABSTRACT

Polyamines occur in plant cells as free molecular bases and they also occur in conjugated form associated with small molecules like phenolic acids or with larger molecules like proteins. Polyamines are mostly conjugated to cinnamic acids e.g., Feruloyagmatine, Ferloyl-3-methoxy tyramine, Octopamine etc. Several studies have shown that the accumulation of Hydroxy cinnamic acid amides (HCAA) result of incompatible plants-pathogen interactions and they have also been shown to exhibit direct antifungal properties[1-3]. Since the plant *Aegle marmelos* Correa (Rutaceae) has been rich source for cinnamic acid amides, we have re-examined this much investigated plant to study their antifungal activity. We here present the isolation, characterization, chemical transformation of alkaloidal amides and their antifungal activity.



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Poster Presentations

Allelochemicals as novel molecules for developing environmentally benign herbicides

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ABSTRACT

Allelochemicals are chemicals found in plants that suppress the growth of other plants upon release in the environment resulting in a natural phenomenon known as *allelopathy*. These chemicals exhibit great diversity in chemical nature and are biologically active. Besides being inhibitors of growth, these also possess species specificity and thus hold a good promise as chemicals of herbicidal interest. They are biodegradable and possess unique molecular target sites different from the known herbicides. In view of the ill-effects of synthetic herbicides on human health and environment, the use of safer chemicals constitutes one of the exciting fields of agrochemical research. For weed management allelochemicals can be used following a variety of strategies. These can be used directly like the commercially available herbicides e.g. essential oils, sorgoleone (from *Sorghum* sp.), sesquiterpene lactones like artemisinin and parthenin, and quassinoids. Secondly, these can serve as templates for the synthesis of novel natural plant-based herbicides, e.g. monoterpenes like cineole and leptospermones from *Callistemon* sp. Further, crop cultivars can be improved through biotechnological approaches such as DNA recombinant or transgene technology by introducing genes that encode synthesis of potential allelochemicals. For this, crop plants with high allelopathic activity are identified through germplasm screening. This paper discusses the potential of allelochemicals as novel compounds for sustainable weed management.

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Poster Presentations

Antioxidant activity, total phenolic and flavonoid content of bottle brush (*Callistemon viminalis*)

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ABSTRACT

Reactive oxygen species (superoxide, hydroxyl, hydrogen peroxide and singlet oxygen etc.) produced as by-products of normal metabolic activities are chemically reactive ions that cause oxidative damage to enzymes, carbohydrates, proteins and lipids. Living cells normally protect themselves by scavenging these reactive free radicals. However, due to increased exposure to pollutants, tobacco smoke, ionizing radiations, synthetic pesticides and solvents, their production increases manifold. Living cells are unable to scavenge these increased levels of free radicals. It has necessitated the inclusion of synthetic antioxidants in food stuff but the latter has certain toxicological concerns linked to their use. As a result, the focus has shifted towards natural sources of antioxidants that are safer to use. In this direction, aromatic plants and their products hold good potential. *Callistemon viminalis* (Myrtaceae) is one such tree that has been investigated in this context. We evaluated the aqueous leaf extracts (0.5 – 5%) and leaf essential oil (50 – 400 μg/ml) and its two main components- 1,8-Cineole and α-pinene (50 – 400 μg/ml) for antioxidant activity against $NO^{\cdot}$ radical and H_2O_2 and reducing power using ferric reducing antioxidant power (FRAP) assay. NO scavenging activity ranged from 9.1% - 63.6% for water extracts, 14% - 41% for *Callistemon* oil and 52.3% - 69.6% for α-pinene. Likewise, the H_2O_2 scavenging activity and reducing power of aqueous extracts was significantly higher and parallel to the commercial antioxidant BHA. However, the FRAP activity of essential oil and α-pinene was 10.7 - 50% for *Callistemon* oil and 6.8% -31% for α-pinene. The aqueous extracts were found to be rich in phenolics (0.80 μg/mg) and flavonoids 2.8 μg/mg. Based on these results, it is concluded that leaves of *Callistemon* possess free radical scavenging activity and thus could be used as natural antioxidant.

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Poster Presentations

In vitro radical scavenging and antioxidant activities of the essential oil from *Eucalyptus* species

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ABSTRACT

Eucalyptus is a large genus of tall evergreen trees that are extensively planted throughout the world for pulpwood. Additionally, the tree leaves are harvested for the essential oil that is used in food, flavour, and perfumery industry. The present work investigated the antioxidant and free radical scavenging activities of essential oils from the leaves of two *Eucalyptus* species (*E. citriodora*, and *E. tereticornis*) in terms of DPPH radical, hydroxyl radical, nitric oxide, and superoxide anion scavenging activity. Eucalypt essential oil (50- 400 µg/ml) exhibited strong total antioxidant activity showing 28–98%, 15–67%, and 13–70% scavenging of DPPH, hydroxyl, and superoxide radicals, respectively. The essential oil from *E. citriodora* showed greater radical scavenging activity than *E. tereticornis* oils. The radical scavenging and antioxidant properties of the oils were greater than those of commercial antioxidant BHT/ascorbic acid. Further, we evaluated the radical scavenging activity of citronellol, cineole and citronellal - the major constituents of eucalypt essential oil. However, the antioxidant activity of these oils was much lesser than that of essential oils. The results indicate that volatile oils from *Eucalyptus* spp. are a good source of naturally occurring antioxidants for use in food preservation and in pharmaceutical industry.

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Poster Presentations

Synthesis of quinazolinon-2-yl-tetrasubstituted thiophenes as modulator of NF-kB & AP-1 transcription factors

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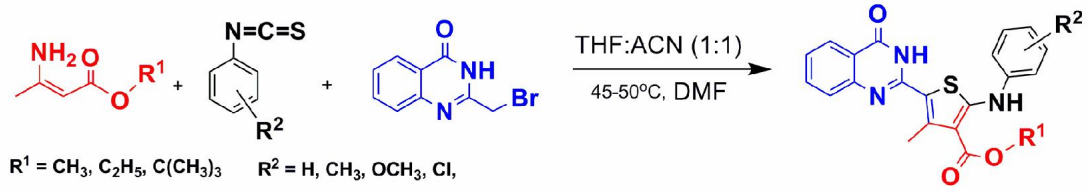
ABSTRACT

Quinazolinone and quinazoline scaffold are class of fused heterocycles that are of considerable interest because they possess diverse range of biological properties. The quinazoline moiety is known to have inhibitory effects on receptor tyrosine kinases, which are promising targets in cancer chemotherapy which includes approved drugs like erlotinib, lapatinib, gefitinib etc. In addition to this, quinazolin-2-yl-thiophenes have been found to be inhibitors of NF-kB and AP-1 proteins[1]. NF-kB proteins are a class of 'rapid-acting' transcription factors that regulate the expression of more than 400 target genes and play a pivotal role in several important physiological processes including immune and inflammatory responses[2]. These transcription factors have been known to be an important link between inflammation and cancer. Inhibition of NF-kB and AP-1 are known to inhibit cancer[3]. However, compared to inhibitors, specific NF-kB activators are less well studied. Recent findings suggest that activating NF-kB, under certain circumstances, may be useful in cancer therapy, radiation protection[4] and anti-HIV treatment[5]. In order to obtain structurally diverse molecules with better biological activity, we have designed and synthesized various quinazolin-2-yl-tetrasubstituted thiophene compounds using a versatile one-pot multicomponent synthesis approach for the novel quinazolin-2-yl-tetrasubstituted thiophenes[6]. These complex molecules were synthesized readily in a one step instead of traditional multi-steps synthesis as shown in the Scheme 1. These molecules were then subjected for the screening of NF-kB and AP-1 in-vitro biological assay. The results of screened compounds for NF-kB and AP-1 activation have shown reasonably good activation of these transcription factors. Compound PMCHJ-1B, PMCHJ-3B, PMCHJ-9B, PMCHJ-10B, PMCHJ-11B and PMCHJ-12B were found to be the activator of either NF-kB or/and AP-1 transcriptional activities. The compound with enhanced NF-kB and AP-1 activation can be useful as radioprotection agent in the cancer chemotherapy, where the normal cells are affected by radiation. These results may be useful for further design and development of compounds with better radioprotection activity in cancer.



Scheme 1: One-pot synthesis of 4-substituted quinazolinon-2-yl-tetrasubstituted thiophenes

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Poster Presentations

Design and synthesis of bis-heterocycles as novel ligands for selective adenosine receptor subtypes

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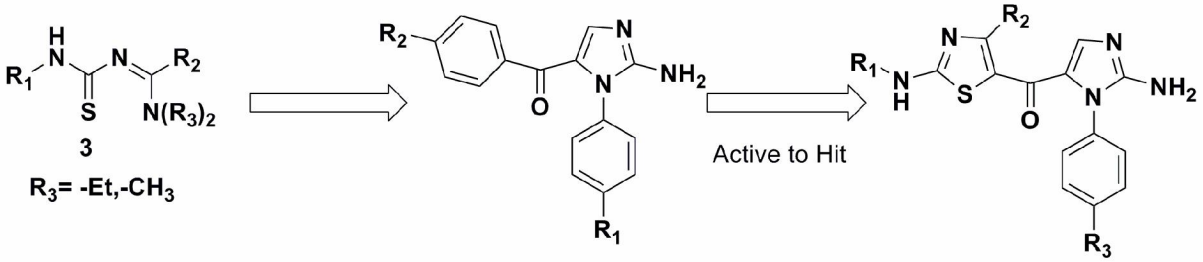
ABSTRACT

Receptors for adenosine are currently of great interest as targets for therapeutic intervention due to their ubiquitous distribution throughout the body and their important modulatory effects on cell function. Adenosine mediates its effects through specific G-protein-coupled receptors ubiquitously expressed in the body and classified as A_1, A_{2A}, A_{2B} and A_3 (ARs). It is believed that the activation of the A_{2B}/A_3 AdoR on human lung mast cells leads to mast cell degranulation, releasing inflammatory cytokines (IL- 4, IL-8, and IL-13) which are responsible for the Asthma and COPD. The inhalation of adenosine causes bronchoconstriction in asthmatics, but not in normal subjects, and there is a significantly higher concentration of adenosine in the bronchoalveolar lavage fluid of asthma sufferers compared to normals.Thus, to develop a dual adenosine A_{2B}/A_3 receptor antagonist would be interesting for the intervention of asthma and COPD[1]. We are particularly interested in the role of adenosine as a mediator in allergic asthma, an area which is currently receiving renewed attention. Several efforts have been devoted to develop potent and selective dual human adenosine A_{2B}/A_3 receptor antagonists which have resulted xanthine based ligands. The problem associated with the xanthine based ligands is its low solubility and bioavailability. Thus, there is need for the non-xanthine based ligands with selectivity to the adenosine receptor subtypes. We here report the designed and synthesis of conjugated 2-aminoimidazole – 2-aminothiazole derivatives as dual adenosine A_{2B}/A_3 receptor antagoinist. The key step involves the reaction of a building block (2-chloroacetyl) thiazoles with amidinoguanidine proceeding through C-C bond formation via 5-*Exo-Trig* cyclization.



Scheme 1: Retrosynthetic analysis and designed of the molecules.

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Poster Presentations

Novel synthesis, characterisation and activity predication of some new class of hydroxytriazenes incorporating antipyrine moiety

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ABSTRACT

Computer aided drug designing has recently attracted attention of synthetic organic chemists. PASS (Prediction of Activity Spectra for Substances) is a very simple tool for prediction probable activity theoretically on the basis of molecular structure. In the present investigation four hydroxytriazenes namely 3-hydroxy-3-(3-methyl phenyl)-1-(4,5-dimethyl-3-phenyl-3,4-dihydro-3H-pyrazol-2-one-1-yl)-triazene, 3-hydroxy-3-(4-methyl phenyl)-1-(4,5-dimethyl-3-phenyl-3,4-dihydro-3H-pyrazol-2-one-1-yl)-triazene, 3-hydroxy-3-(4-chloro phenyl)-1-(4,5-dimethyl-3-phenyl-3,4-dihydro-3H-pyrazol-2-one-1-yl)-triazene and 3-hydroxy-3-[4-(hydroxymethyl) phenyl]-1-(4,5-dimethyl-3-phenyl-3,4-dihydro-3H-pyrazol-2-one-1-yl)-triazene bearing an antipyrine moiety have been synthesized by coupling of aryl hydroxylamine obtained by reducing substituted nitrobenzenes with diazonium salt obtained from 4-amino antipyrine taking hydroxyl amine in excess at the temperature between 0-5°C. The product of coupling was washed and crystallized using appropriate solvent. Their chemical structure was confirmed by IR, ^{1}H NMR, MASS and by elemental analysis. Synthesized compounds have been screened using PASS (http://www.ibmh.msk.su/PASS) for probable activities and good antiviral, antipyretic activity along with number of other activities have been predicted. However these have to be validated by experimental bioassay. The present paper thus paves way for CADD.

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Poster Presentations

Heterocyclic scaffolds via cycloaddition reactions of allylamines

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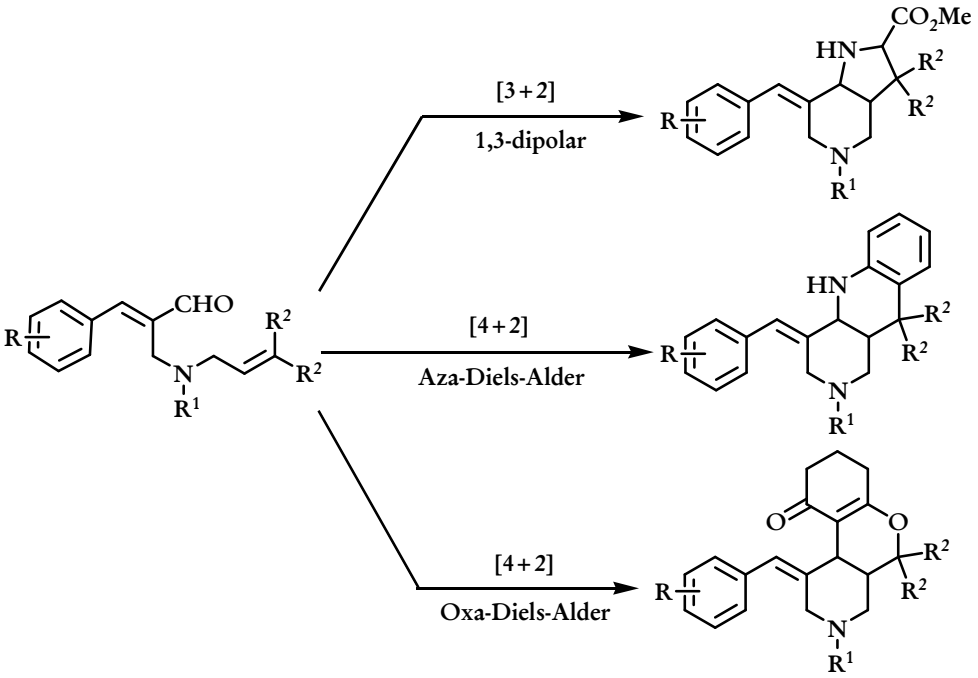
ABSTRACT

Intramolecular cycloaddition reactions with high regio and stereocontrol are important tools for the synthesis of diverse heterocyclic scaffolds[1]. In our pursuit to exploit the substrates generated from the Morita-Baylis-Hillman for heterocyclic synthesis, we have demonstrated that the substituted allylamines afforded from the MBH adducts are suitable precursors to annulated triazoles and tetrazoles via cycloaddition reactions[2]. In continuing program, we have now synthesized substituted 2-formyl allylamines and explored its potential for heterocyclic synthesis via different cycloaddition reactions. Subjecting substituted 2-formyl allylamine to [1,3] dipolar cycloaddition reaction in the presence of amino acids afforded the pyrrolo-piperidine framework whereas [4+2] cycloaddition reaction with aniline (Aza-Diels Alder) and 1,3-cyclohexanedione (Oxa-Diels-Alder) resulted in pyrano-piperidine and benzo-napthyridine frameworks, respectively. The details of the results and stereochemical issues of the synthesized products will be presented and discussed.



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Poster Presentations

Design and synthesis of new pyranone-based hepatoprotectants as anti-hyperglycemic agents

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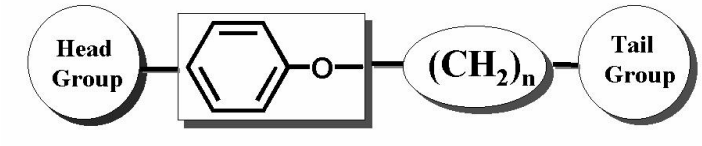
ABSTRACT

Type-2 diabetes is a polygenic and progressive metabolic disorder characterized by insulin resistance, hyperglycaemia, hypertriglyceridaemia, and low plasma HDL-cholesterol[1]. The thiazolidinediones (TZDs, also known as "glitazones") are effective insulin sensitizers and have been shown to improve glucose uptake and lower hyperglycaemia and hyperinsulinaemia[2]. Pioglitazone and rosiglitazone are two marketed PPARγ selective agonists for the treatment of diabetes, which are in clinical use since 2000. In addition, several phenyl acetic derivatives have also been reported to activate PPARs both in vitro and in vivo[3]. However, side effects such as risk of hepatotoxicity, heart failure, edema, fluid retention, and weight gain in patients treated with these drugs warrant development of newer drugs with better pharmacological and safety profiles[4]. Thus, considering the legitimate affinity offered by TZD class of compounds towards PPARγ, we envisaged that transformation of a known hepatoprotectants into TZD-based PPARγ agonists would be an interesting undertaking for identification of new safe anti-hyperglycemic leads. Studies have shown that polysubstituted 2-pyranones possess significant hepatoprotective activity as well as anti-hyperglycemic activity [5]. After examining various known hepatoprotectants, their biological activity and information from co-crystal structure of PPARγ, we designed and synthesized new pyranone-based TZDs and phenyl acetic acid derivatives as insulin-sensitizing agents. Encouraging results have been obtained and further biological studies of these compounds are currently underway.



Basic ligand structure for PPARγ

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Poster Presentations

Comparative QSAR studies of imidazopyridazine derivatives using theoretical structural properties

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ABSTRACT

Quantitative Structure–Activity Relationship (QSAR) studies have been carried out on a series of 35 recently synthesized imidazopyridazine derivatives to find out the structural requirements of their inhibitory activity against malarial kinase PfPK7. The statistically significant best 2D QSAR model having correlation coefficient r^2 = 0.9190 and cross validated squared correlation coefficient q^2 = 0.8575 with external predictive ability of pred_r^2 = 0.7212 was developed by stepwise partial least squares regression (SW-PLSR) method with the descriptors like StNE-index, T_N_O_2, T_N_O_7, YcompDipole and SaasCE-index. The 3D-QSAR studies were performed using the stepwise variable selection k-nearest neighbor molecular field analysis approach (SA kNN-MFA); q^2 of 0.8422 and pred_r^2 of 0.5836 were obtained. It uses one steric and three electrostatic fields along with its 5*k* nearest neighbor (*k*=5) to evaluate the activity of new molecules. The results of the present study may be useful on the designing of more potent imidazopyridazines as PfPk7 inhibitors.

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Extraction and studies of '*Citrus medica*'-A potent medicinal plant in the Kachchh region

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ABSTRACT

Kachchh is a land with great value of medicinal plants. Some of them are having wild range of applications. We have chosen a plant with having a great value in religion as well as medicinal since ancient to current Indian generation. In this reference we have selected to study its medicinal values. Citrus fruits and juices have long been recognized to contain secondary metabolites including antioxidant such as ascorbic acid, flavanones, phenolics and pectin that are important to human nutrition. Studies have found antioxidant in juice and edible parts of oranges of different origin and from different varieties. In this aspect we have extracted juice and separated edible parts and evaluated the chemical parameters and studied their medicinal value. The method for extraction and investigation of ascorbic acid has been studied. Others physical data have been obtained and analyzed.

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Poster Presentations

New thermal stable homo-polymers of 4-sulfonamide phenyl maleimide and 4-azophenyl N-phenyl meleimide: Synthesis and their characterization

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ABSTRACT

Two new thermal stable homopolymer H-PSPMI, H-PAPI of 4-sulfonamide phenyl maleimide and 4-azophenyl N-phenyl maleimide monomer were synthesized respectively using a free radical monomer initiator azobisisobutyronitrile (AIBN). Monomers were synthesized using 4-aminobenzene sulfonamide, 4-phenylazo aniline, maleic anhydride in DMF solvent. Monomer and homopolymers were characterized by FT-IR and ^{1}H-NMR spectroscopy. Thermal behaviour was studied by Thermogravimatric analysis (TGA). The molecular weights of homopolymers were determined by gel permeation chromatography (GPC).

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Poster Presentations

Synthesis, characterization, copolymerization of 3-Cl 4-F (phenyl) maleimide with MMA and study of antimicrobial activity

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ABSTRACT

The copolymer of 3-Cl 4-F (phenyl) maleimide (N-CFPMI) with methylmethacrylate (MMA) were prepared free radically at 70°C using Tetrahydrofuran (THF) as a solvent and Benzoyl peroxide (BPO) as a free radical initiator. Obtained homopolymer and copolymer were characterized by intrinsic viscosity, solubility test, FT-IR and ^{1}H-NMR spectroscopy. Variations in yield based on solvent, free radical initiator and time was also studied. The molecular weight of copolymer was determined by gel permeation chromatography (GPC). Thermogravimetric analysis (TGA) characterizes the thermal behaviour of polymer. The antimicrobial activity is also analysized.

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Poster Presentations

Synthesis, characterization homopolymer and copolymer of 2-chloro 4-nitro (phenyl) maleimide with MMA

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ABSTRACT

The homopolymer and copolymer of 2-Chloro 4-nitro (phenyl) maleimide (N-OCPNPMI) with methylmethacrylate was prepared free radically at 70°C using Tetrahydrofuran (THF) as a solvent and Benzoyl peroxide (BPO) as free radical initiator. Resulting homo and copolymer was characterized by intrinsic viscosity, solubility test, FT-IR, ^{1}H-NMR spectral analysis. Effect of solvent, free radical initiator, time on polymers yield was also studied. The molecular weight and polydispersity index was determined by Gel permeation chromatography (GPC). The thermal stability of homopolymer (H-OCPNPMI) and copolymer (C-OCPNPMI1) was determined by Thermogravimetric analysis (TGA) characterizes the thermal behaviour of polymers.

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Poster Presentations

Synthesis, characterization and study on antimicrobial activity of copolymer of 4-chloro (phenyl) maleimide with MMA, EA

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ABSTRACT

The copolymer of 4-Chloro (phenyl) maleimide (N-PCPMI) with methylmethacrylate (MMA) and ethyl acrylate (EA) was prepared free radically at 70°C using THF as a solvent and BPO as a free radical initiator. Obtained copolymers were characterized by density measurement, intrinsic viscosity, solubility test, FT-IR, ^{1}H-NMR spectral analysis. Variations based on solvent, free radical initiator, time was also studied. Thermogravimetric analysis (TGA) characterizes the thermal behaviour of polymers, gel permeation chromatography (GPC) was done for the determination of number average molecular weight, polydispersity index. The antimicrobial activities of copolymers were also investigated against various microorganisms.

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Poster Presentations

Investigation of the physiological properties and synthesis of PUFAs from thraustochytrids and its electrophoretic karyotypes

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ABSTRACT

Polyunsaturated fatty acids (PUFAs) play an important role in various biological functions such as inflammatory response, brain development, reducing heart disease and improving vision sensitivity. Fish have been the major natural sources for the synthesis of PUFAs, but in recent years its production has declined. Therefore, there is an interest in obtaining economically important PUFAs from other alternative and sustainable sources. In this present study, physiological properties of organism, such as the number of chromosomes, genome size, fatty acid profile and the activities of desaturases and elongases were investigated for four different *Thraustochytrium* species. The investigation revealed that *Thraustochytrium aureum* could synthesize a significant level of PUFAs, particularly docosahexaenoic acid (DHA), when compared to the other three *Thraustochytrium* species tested. A higher level of saturated fatty acids was observed by *T. striatum* followed by *Thraustochytrium* sp. ATCC 26185. The PUFA accumulation rate was higher in the n-3 than in the n-6 pathway. A comparison of the activities for these desaturases and elongases of the four different species were also studied. Further, the electrophoretic karyotypes of Thraustochytrids were separated by pulsed-field gel electrophoresis (PFGE). The separation condition of PFGE was developed to obtain the different chromosomes from the *Thraustochytrium* species. The number of chromosomes in *T. aureum, T. striatum, Thraustochytrium* sp. ATCC 20891 and *Thraustochytrium* sp. ATCC 26185 were 13, 17, 10, 8, and the whole genome size of those species were estimated to be 12.9, 11.7, 11.3, and 9.93 Mbp, respectively.

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Poster Presentations

Shelf life evaluation of an effective ant repellent from hyptis suaveolens

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ABSTRACT

Hyptis suaveolens, (family: Lamiaceae) commonly known as bushmint is considered as a weed plant of plains. It grows very fast and suppresses most of the vegetation present in its surrounding. Despite use in traditional system of therapy and exhibiting antimicrobial, antinflammatory, antifungal, antioxidative proprties the plant is non palatable to animals and not being utilized for any potential therapeutic development and considered as complete waste plant. Having strong aromatic property it has been identified for many phytochemicals like alkaloids, flavonols, flavones, flavonones, terpenoids, tannins, aldehydes and ketones, but application of this plant is still unrecognized. We have reported its insect repellent activity and in present study reporting its specific ant repellent property with aqueous extract along with its shelf life. 5% (w/v) aqueous extract was prepared from shed dry leaves. Extract was filtered and stored at room temperature. White A4 sheets were whipped both side with 5.0, 2.5, 1.25 and 00 % extract. After being airdry the sheets were placed on a surface, some food material was spread on it to attract the ants. The sheets were monitored for comparative aggregation of ants on food substance. After 2 hrs it was found that no ants were attracted on any of the concentration of Hyptis execpt for the control i.e. 00%. Camera recording was done to enumerate the results. To check the shelf life of extract 60 and 30 days old extracts were used along with fresh one and was found that all stored extracts restored the similar repellent efficacy for ants.

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Poster Presentations

Synthesis of modified nonionic thioacetamido-linked dimer of LNA of biological importance

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ABSTRACT

The last two decades have witnessed an upsurge in the synthesis of several modified nucleic acid derivatives. The intentions have been to synthesize therapeutically suitable and commercially viable nucleic acid analogues. Oligonucleotide-based antisense strategies represent a unique paradigm for the treatment of a wide variety of human diseases states. The novel utility of these agents resides in their ability to selectively prevent the expression of a particular disease-associated gene in a sequence specific manner. Successful drug development based on this technology requires the synthesis and use of chemically modified oligonucleotides that render stability to nucleolytic digestion, enhance cellular uptake, and hybridize with high affinity and specificity toward the target mRNA. Ongoing synthetic studies into this broad class of compounds have focused on the chemical modification of the backbone, sugar, and base functionalities of natural DNA.[1-7] We have designed and synthesized the five atom thioacetamido-linked LNA based dimers I, II, III and IV mentioned in (Figure 1). The detailed synthetic scheme will be presented during the poster session.

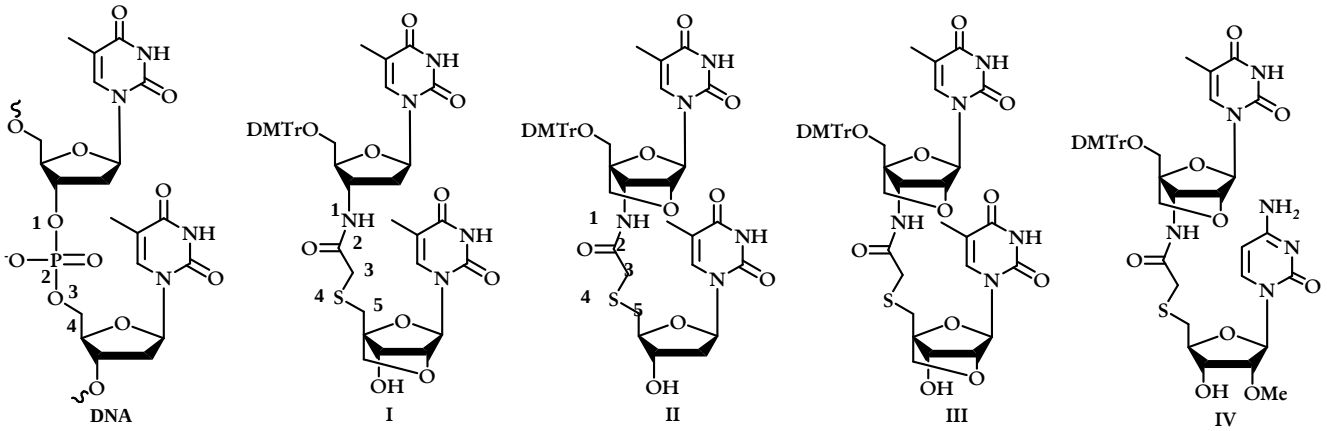

Figure 1

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Poster Presentations

Synthesis of *N*-acylated-7-amino-4-alkyl/aryl coumarin derivatives and evaluation of their Src kinase inhibitory & anticancer activities

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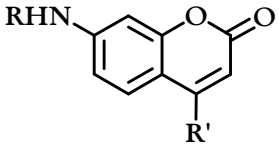
ABSTRACT

Numerous biological activities have been attributed to coumarins and their analogs. It has been long recognized to posses anti-inflammatory, anti-oxidant, anti-allergic, hepatoprotective, anti-thrombotic, antiviral and anticarcinogenic activities. Moreover, aminocoumarins belong to a class of antibiotics, which act by an inhibition of DNA Gyrase enzyme involved in the cell division in bacteria and also found application, as photo sensitizers, optical brightening agents and as additives to fibers and paper. According to the World Health Organization, cancer causes 13% of deaths worldwide. Src Kinase belongs to a class of protein tyrosine kinase (PTK) and has been implicated in the genesis and progression of multiple types of human cancer including colon, breast, lung, and other cancers. Thus, designing Src kinase inhibitors is a subject of major interest by pharmaceutical industry. Our own interest and also the stimulating background of coumarin derivatives, prompted us to synthesize a series of 7-amino-4-alkyl/aryl coumarins and their N-acylated derivatives. All these compounds were screened for their inhibitory activity against Src kinase and anticancer activity on human breast carcinoma cells, BT-20 cell line.The details of the work will be presented in poster.



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Poster Presentations

Synthesis and platelet aggregation inhibition activity evaluation of *o*- and/ *N*-acylated dihydropyrimidinones

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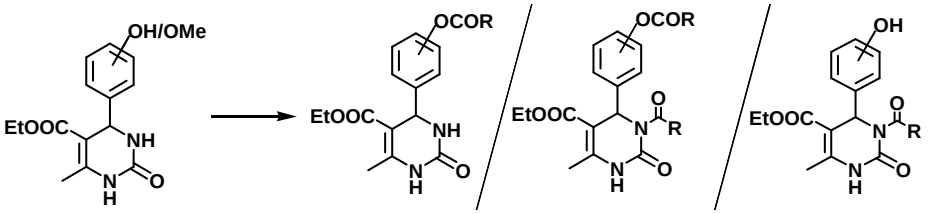
ABSTRACT

In the recent past, new interests have grown up in the antihypertensive agents having calcium channel blocking activity for the prevention of platelet aggregation. More recently, appropriately functionalized dihydropyrimidinone derivatives have emerged as potent calcium channel blockers, antihypertensive agents and α_{1a}-adrenergic receptor selective antagonists. Investigations of dihydropyrimidinone compounds for their pharmacological activities against cardiovascular diseases have already begun but they have not been explored much as antiplatelet agents. We report in the present work the synthesis of differently acylated DHPMs with increasing acyl group chain length and also varying the position of acyl chain on the aryl DHPM scaffold. All the synthesized dihydropyrimidinone compounds have been investigated for platelet anti-aggregation activity as % inhibition of ADP induced platelet aggregation by virtue of calcium channel blocking (CCB) activity and intracellular enahancement of nitric oxide (NO) level. We acknowledge the financial support from the University of Delhi (DU-DST Purse Grant) for this research work.



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Poster Presentations

Characterization of potential phosphate dissolving bacterial culture isolated from sugar cane rhizosphere

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ABSTRACT

Phosphorus is the second important plant nutrient after nitrogen Donahue et al[1]. Phosphorus availability is low in soils because of its fixation as insoluble phosphates of iron, aluminum and calcium. Phosphorus supply through biological means is a viable alternative; phosphate solubilizing microorganisms (PSM) are active in conversion of insoluble phosphate to soluble primary and secondary orthophosphate ions Gyaneshwar et al[2]. Numerous microorganisms, especially those associated with roots have the ability to increase plant growth and productivity Chang et al[3]. Phosphate solubilizing bacterium isolated from sugar cane rhizospheres Chakkarvarthy et al[4] as SVM 18 was characterized in the present research work. Potential use of this bacterium as bioinoculant depends exclusively on growth conditions. Its physiological and biochemical characterization was done by various methods like soluble phosphorus estimation M L Jackson[5], phosphatase estimation Bhattacharjee et al[6], growth curve, effect of P^H, temperature and salt concentration on growth, different biochemical characterization, and antibiogram studies as well as determination of N_2 fixing abilities. Biochemical characterization was also done using GC-MS Sharif et al.[7] and API. Isolated culture has good potential as phosphatic biofertilizer.

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Poster Presentations

'Bhal' wetland flora - Biodiversity, mineral composition and their relationship

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ABSTRACT

Gujarat has a coastal belt of approximately 1600 km and has exclusively diversified species. 'Bhal' region is situated on the south-west border of Saurashtra, spreading in 2 revenue districts of Bhavnagar and Ahmedabad on the left border of the Gulf of Khambhat (Cambay). Studies on coastal flora have assumed a new dimension in recent years because of their utility as human food (vegetables, salads, pickles); fodder (for camels, sheep, goats, wild life and fish); wood for building materials; bio-fuel, chemicals, landscaping and dune stabilization. In present investigation attempts have been made to study the relation ship between biodiversity and mineral composition in the leaves of dicotyledonous and monocotyledonous species. Accumulation of Na^+, Cl^-, Mg^{2+}, K^+ and ash content in leaves of 3 dicotyledonous (*Suaeda nudiflora*, Moq., *Prosopis chilensis,* Stunz. and *Salvadora persica*, Linn.) and 3 monocotyledonous (*Aeluropus lagopoides*, Linn., *Sporobolus coromandellianus*, Link and *Schoenoplectus maritimus*, Lye.) species have been analysed. The data were subjected to 2-way ANOVA and *t-test* before making justifiable conclusions.

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Characterization of a diesel-degrading strain isolated from hydrocarbon-contaminated site

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ABSTRACT

A diesel-degrading bacterium has been isolated from a diesel-polluted site. The isolate was tentatively identified as *Pseudomonas aeruginosa* strain based on Bergey's manual of bacteriology. Bushnell Haas (BH) broth containing 1 per cent diesel was used as selective medium. Isolate showed an almost linear increase in cellular growth with respect to diesel concentrations with optimum growth occurring at 4% (v/v) diesel concentration. The optimal pH that supported growth of the bacterium was between 7.5 to 8.0 and the isolate exhibited optimal broad temperature supporting growth on diesel from 27 to 37 °C. An almost complete removal of diesel components was seen from the medium was also reported. The characteristics of this bacterium suggest that it is suitable for bioremediation of diesel spills and pollutions in the tropics.

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Poster Presentations

Photocatalytic bleaching of evans blue over zinc oxide particulate system

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ABSTRACT

The effluents from dyeing and printing industries when discharged into river, ponds, etc., not only disturb the ecosystem but also pose a serious health hazard for the human beings. With the increase in the environmental awareness all over the world, search for new cost effective and green routes for treatment of water contaminated with dye effluents have been accelerated in last two decades. Advanced Oxidation processes (AOPs) and technologies (AOTs) are characterized by the production of short lived chemical species of high oxidation power especially the hydroxyl radical. Heterogeneous photocatalysis is one of the promising AOTs to treat polluted water and it attracted the attention of scientific community all over the world[1,2]. Most commonly used semiconductors (Photocatalyst) in heterogeneous photocatalytic process are TiO_2 and ZnO, however, the colored semiconductors have also been investigated for treatment of water to harness solar energy[3]. Photocatalytic bleaching of Evans blue (an azo dye) has been investigated in presence of zinc oxide particulate system. Controlled experiments were carried out to establish the nature of the process. It was observed that the reaction is photocatalytic in nature. The progress of the reaction was monitored spectrophotometrically. A 500 W tungsten lamp was used as a light source in the present investigation. The effect of various parameters likes concentration of the dye, pH, amount of semiconductor, light intensity, etc. on the rate of photocatalytic bleaching was studied and optimum conditions were obtained. During the photocatalytic degradation, the photocatalyst (Zinc Oxide) remains unaffected which was confirmed from its FT-IR spectrum. On the basis of the experimental observations, a tentative mechanism for the photocatalytic bleaching of Evans blue has been proposed.

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Poster Presentations

Synthesis and anti cancer activity of some new 1,4-dihydropyrimidine derivatives

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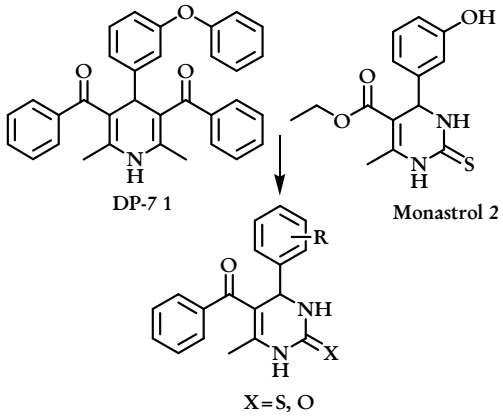
ABSTRACT

3,5-Dibenzoyl-1,4-dihydropyridine (DHP) derivative, DP-7, emerged as a potent multidrug reverting agent that inhibits efflux of drug from cell wall by inhibiting activity of ATP Binding Cassettes (ABC). On the other hand, dihydropyrimidine (DHPM) derivative, (aza analogue) namely, monestrol inhibits the Eg5 protein responsible for the separation of daughter chromosomes during cell division and controls the growth of tumor cells. these two potent molecules have been hybridized to get the duel action in cancer chemotherapy by synthesizing various thio and oxo analogues, bearing variety at 4th position of the DHPM ring (Scheme-1). The newly synthesized molecules were screened for anti cancer activity.



Scheme 1

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Poster Presentations

Analytical method development for the estimation of iridoid glyoside from leaves of vitex negundo

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ABSTRACT

Vitex negundo (verbenaceae) is a reputed medicinal herb and its parts have been employed as a traditional cure in Asian systems of medicine (Indian, Chinese, Malaysian) for a variety of disease conditions. A number of pharmacological activities have been attributed to V. negundo. In the present study isolation of an iridoid glycoside (negundoside) from leaves of V. negundo has been carried out. Also validated RP-HPLC analytical method has been developed for its estimation in crude drug. Separation was achieved on ODS column with acetonitrile:water (25:75 v/v) mobile phase. Detection was carried out using UV detector at 260 nm. Linearity in the response of negundoside was observed in the concentration range 0.8 - 40 μg/mL with correlation coefficient of 0.9994. The recovery of the compound was between 96.3–101.5%. The relative standard deviations was ranged between 1.53–1.81 (Intra-day) and 1.33–1.96 (Inter-day). The methods can be used for routine analysis of the negundoside content in the crude drug as well as extract of the plant.

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Poster Presentations

In vitro evaluation of wound healing efficacy of plant extracts containing beta-sitosterol on HaCaT cells and its validation using rat model

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ABSTRACT

Wound healing is the process which involves highly integrated series of cellular, physiological and biochemical processes. Several factors delay or reduce wound healing including bacterial infection, necrotic tissue, interference with blood supply etc. If above factors could be altered by any agent, an increased healing rate can be achieved. Plants have been used as traditional wound healers since ancient times as a practice in traditional medicine for all kinds of wounds. The wound healing efficacy of plants is attributed to phytochemicals produced naturally in plants as their defense mechanism against various kinds of stress the plants are put to by nature or physically. It has also been reported that there are several plants used in wound healing activity which consists of various agents that can alter factors resulting in good and faster wound healing activity.The phytoconstituents which help in the wound healing activity and which are present in these plants are Sterols (Beta-Sitosterol), Triterpenes (Lupeol) and flavanoids (Flavonol), Phenols (Gallic Acid). Limonia acidissima, Blumea lacera and Tridax procumbens extracts were made and the Beta-Sitosterol content in this plant extracts were estimated by proliferation and migration assay on HaCaT cells in vitro. In Current study HaCaT cells were treated with plant extracts with concentrations (5 μg/ml, 25 μg/ml and 100μg/ml). There was significant increase in cell migration and proliferation in comparison with the control. The results suggest that plant extracts enhance directly the rate of invitro migration and proliferation of HaCaT cells indicating enhanced keratinocyte viability resulting in wound healing. The in vitro results are validated using the rat model for burn wounds.

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Poster Presentations

Synthesis of 2-aminoimidazole alkaloids from propargylamines and thiourea

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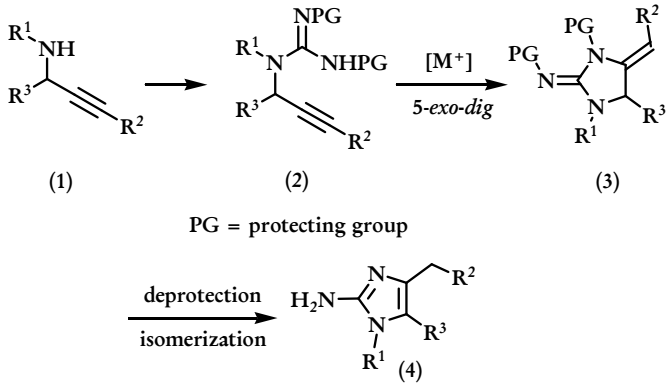
ABSTRACT

The 2-aminoimidazole unit is emerging as an important pharmacophore and is widely found in numerous biologically active marine sponge alkaloids. A large number of these alkaloids, isolated from *Leucetta sp.* (class Calcarea), has been shown to exhibit a diverse range of biological activities around a relatively small structural core, thus providing an important scaffold for both medicinal and discovery based research. Herein we describe a novel, short and efficient synthesis of several natural 2-aminoimidazoles from *Leucetta sp.* as well as their analogues starting from readily available polysubstituted secondary propargylamines and thioureas[1-3] (Scheme-1).



(1) (2) (3) (4)

Scheme 1

REFERENCES

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Poster Presentations

Synthesis and pharmacological evaluation of 2,5-disubstituted-1,3,4-thiadiazoles

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ABSTRACT

The penicillins, cephalosporins, macrolides, tetracylcines, aminoglycosides, and chloramphenicol were all recognized to be therapeutically effective antimicrobials between 1940 and 1975. Despite this, no major therapeutic group of agents has been identified through natural product screening in the last quarter of the century. Further the development of widespread resistance to the existing agents has created an urgent need for new antimicrobial agents. Intense investigation is being carried out on thiadiazole compounds owing to their wide spectrum of activity. The different classes of thiadiazole compounds are 1,2,4-thiadiazoles; 1,3,4-thiadiazoles and 1,2,5-thiadiazoles. Amongst these 1,3,4-thiadiazoles represent the most therapeutically active class of compounds and have wide range of biological activities. Intermediates, different Schiff bases were obtained by reaction of thiosemicarbazide with suitable aldehydes. These different Schiff bases were reacted with ferric chloride to obtain 5-substituted-2-amino-1,3,4-thiadiazoles. These were again reacted with substituted acid chlorides and 2,5-disubstituted -1,3,4-thiadiazoles were obtained. The structures of the synthesized compounds were established by ^{1}H NMR, mass and IR spectroscopic techniques. The 2,5-disubstituted-1,3,4-thiadiazoles were evaluated for their in vitro antibacterial activity by agar well diffusion technique using soyabean casein digest agar medium against 3 gram-positive and 3 gram-negative bacteria at different concentrations 800 micrograms per 0.1mL, 1000 micrograms per 0.1mL and 1200 micrograms per 0.1mL. Levofloxacin 30 micrograms per 0.1 mL was used as standard drug. 4-chloro-N-(5-(3-nitrophenyl)-1,3,4-thiadiazole-2yl)benzamide, N-(5-(furan-2-yl)-1,3,4-thiadiazole-2-yl)-4-methoxybenzamide and 4-methoxy-N-(5-(4-nitrophenyl)-1,3,4-thiadiazole-2-yl)benzamide showed good activity against *P.aeruginosa*. This provides new ideas for further research in the same direction.

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Poster Presentations

Anticonvulsant activity and biochemical estimation of norepinephrine from *Ficus carica* L. (moraceae) leaves extract in experimental mice

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ABSTRACT

It is estimated that upto 5% of world's population develops epilepsy. There is an increasing demand of herbal products since the clinical applications of modern antiepileptic drugs are limited due to their unwanted side effects. The aim of the present study was to evaluate the anticonvulsant activity of aqueous acetonic extract of *Ficus carica* (AAEFC) Linn. Preliminary phytochemical studies were carried on extract of aerial parts of the plant. Acute toxicity [1] was performed as per OECD guidelines no. 425 and it was found that the extract was safe till 2000 mg/kg. Anticonvulsant activity of AAEFC was studied in male Swiss Albino mice by using Maximal Electroshock (MES) and Pentylenetetrazole (PTZ) induced convulsions. The standard compounds used were phenytoin and diazepam respectively. Also, a 10 day anticonvulsant study was carried out to evaluate its long term effect. Estimation of Norepinephrine (NE) in mouse brain was performed to study the effect of AAEFC on NE levels. Pretreatment with AAEFC (250 and 500 mg/kg, *p.o.*) significantly reduced the duration and increased the latency to seizures in MES induced tonic seizures and PTZ induced seizures as compared to control group. The standard antiepileptic drugs phenytoin and diazepam completely protected the animals from seizures. A 10 day study of anticonvulsant study of AAEFC showed 100% protection against mortality. NE estimation in brain showed significant enhancement of NE levels compared to control group. Thus, *Ficus carica* L. might be a potential candidate for use as an anticonvulsant drug which was confirmed by increased levels of NE.

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Poster Presentations

Synthesis and pharmacological evaluation of anti-inflammatory mutual amide prodrugs

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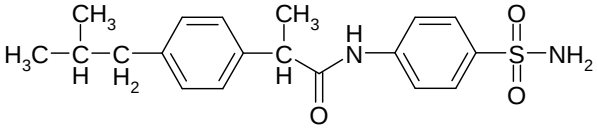
ABSTRACT

Non-steroidal anti-inflammatory drugs (NSAIDs) have been widely used for the management of inflammation, pain and nociception. Gastric intolerance caused by most of the NSAIDs used today restricts their use. Several approaches have been proposed to modify the parent NSAIDs molecule in order to reduce their gastric toxicity [1]. Oral prodrug approach is one of such approaches, which can be applied to ensure safe delivery of NSAIDs [2]. In the present work, commonly prescribed NSAID, Ibuprofen was conjugated with sulfonamides like Sulphamethoxazole and Sulphanilamide via amide bond using dicyclohexylcarbodiimide (DCC) coupling reaction. The products formed were confirmed and characterized by IR and NMR spectras. The synthesized prodrugs were screened for their analgesic and antiinflammatory activity using Eddy's hot plate, acetic acid induced writhing and carrageenan induced rat paw edema methods respectively. These prodrugs were also evaluated for their ulcerogenic potential. All the compounds were found to be less ulcerogenic than their parent NSAIDs and showed better activity profile in terms of analgesic and antiinflammatory activities than their parent drug (Ibuprofen). Amongst all synthesized compounds, compound 2 was found to be most potent. Thus, the synthesized prodrugs exhibited promising analgesic, anti-inflammatory activities and showed less ulcerogenic potential then Ibuprofen. Hence, mutual amide prodrug approach successfully achieved all the objectives of the present work.



Compound 2

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Poster Presentations

Greener and rapid access to some bioactive heterocycles

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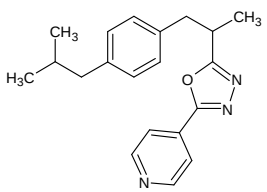
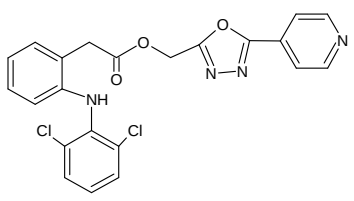
ABSTRACT

The growing ecological awareness has forced researchers to synthesize substances required by society in eco-friendly manner & within short periods of time [1]. The best option to accelerate these synthetic processes is the use of Microwave irradiation [2]. The use of Microwave assisted organic synthesis (MAOS) in synthetic chemistry reduces reaction time and increases product yield. Also, some of the major advances in chemistry have been in the area of catalysts. Modern catalysts provide highly selective routes to synthesize chemical products. Hence, these two methods are considered as Green techniques. The wide occurrence of the heterocycles in natural products has made them important synthetic targets. Their remarkable ability to serve both as biomimetics and reactive pharmacophores has largely contributed to their unique value as key elements of numerous drugs. In the present project some newer 2,5-disubstituted 1,3,4-oxadiazole derivatives of NSIADs (Ibuprofen and Aceclofenac) were synthesized by using two methods, 'Conventional' and 'Greener' method. Conventional method uses $POCl_3$, while greener method uses PbO_2 as a reagent under microwave irradiation. 1,3,4-Oxadiazole moiety was selected for synthesis because of its diverse biological activities. These two methods compared on the basis of the yield, purity and overall green approach of these methods. Synthesized compounds were purified and characterized by suitable chromatographic and spectroscopic techniques. Further they were evaluated for antibacterial, antifungal and analgesic activity. Results of antimicrobial activity are very promising. All compounds showed significant analgesic activity. In fact, the analgesic activity of 4-pyridinyl derived compounds (6e, 6j) was found to be better than that of standard.



Compound 6e



Compound 6j

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Poster Presentations

Tamarind leaf powder supplementation alleviates fluoride toxicity

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ABSTRACT

Fluorosis is a metabolic disease caused by ingestion of excessive amounts of fluoride, mainly through drinking water and food in endemic areas. Fluoride concentrations as low as 0.10 ppm or below to as high as 177 ppm have been reported in natural water resources [1]. Chronic exposure to fluoride results in hyperglycemia, hyperlipidaemia and oxidative stress besides the development of classical symptoms of fluorosis [2, 3]. Chronic fluoride intake is also reported to be diabetogenic [4]. Various defluoridation techniques that are available for removal of excess fluoride from drinking water are expensive and unaffordable by rural population. While there are several reports on the effects of adjuvants (Vitamin C, D, E, calcium, selenium and borate salts etc.) [5-8] that ameliorate fluoride toxicity, the effects of dietary variations have not been investigated. Dietary therapies using plants and plant based formulations have a preventive role in occurrence of cardiovascular disease, diabetes and oxidative stress. It is also known that dietary manipulations are relatively safe with less/ no side effects on normal physiological systems. Tamarind, *Tamarindus indica* L., is a multipurpose tropical fruit tree used for its fruits, which are eaten fresh or processed and used as a seasoning or spice. The leaves, flowers and immature pods of tamarind are edible. The leaves, flowers, fruits and seeds are used to make curries, salads, stews and soups in many countries. The leaves are used to treat throat infections- coughs, fever, intestinal worms, urinary troubles and liver ailments. Leaves and pulp act as a cholagogue, laxative, anticongestant and exhibit anti-oxidant activity in the liver in addition to their blood sugar reducing properties [9]. The present study was undertaken in order to investigate the effects of Tamarind (*Tamarindus indica* L) leaf powder supplementation on carbohydrate, lipid and antioxidant profiles in fluoride exposed (100 ppm sodium fluoride, 4 weeks) male rats. Exposure to fluoride resulted in a significant elevation in plasma glucose and lipid profiles with a reduction in plasma HDL-C content. Inclusion of tamarind leaf powder as a dietary supplement (2.5, 5.0 and 10.0 gm % doses) resulted in significant decreases in plasma glucose as well as lipid profiles and an increase in HDL-C content of the fluoride exposed animals. A significant reduction in hepatic glycogen content, hexokinase activity and an increase in hepatic lipid profiles and G-6-Pase activity were observed in the fluoride exposed rats. Administration of tamarind leaf powder to the diet increased the hepatic glycogen content and hexokinase activities and decreased the hepatic G-6-Pase activities and hepatic lipid profiles in a dose- dependent manner. Excess fluoride in drinking water elevated the hepatic and renal tissue lipid peroxidation and decreased the total ascorbic acid and glutathione contents, superoxide dismutase, catalase, glutathione peroxidase activities in fluoride administered animals. Addition of tamarind leaf powder to the diet reduced the hepatic and renal tissue lipid peroxidation and enhanced the antioxidant profiles significantly. Thus from the present study it is concluded that tamarind leaf powder as an adjuvant mitigates the fluoride toxicity.

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Poster Presentations

Approach of optimization technique in microwave synthesis of novel oxadiazole derivatives

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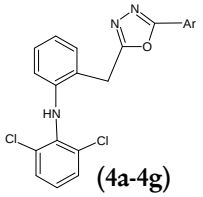
ABSTRACT

The 'Microwave Assisted Organic Synthesis' (MAOS) is more efficient technique than classical water- bath heating, since direct "in-core" heating of the medium occurs. Secondly, microwave heating leads to radically reduced reaction times, higher yields and more pure compounds. The search of novel heterocyclic compounds has led to the discovery of many molecules having tremendous potential. Among nitrogen containing heterocycles, Oxadiazole, nucleus has attracted a wide attention because of its broad biological activities, such as antimicrobial [1], anti-mycobacterial [2], anti-inflammatory-analgesic [3], anti-tubercular [4] etc. Process of drug development and synthesis characterized by utilization of more time, energy and resources and fulfilled through trial and error methods. These issues can be sorted out by the use of technique called as optimization. Lesser experimentations are required to achieve optimum results in Optimization techniques. Optimization techniques comprises of experimental design, mathematical models and graphical outcomes. The present project aims at the synthesis of some newer 2,5-disubstituted 1,3,4-oxadiazole analogues using MAOS method. In sight of this, various oxadiazole derivatives of NSAID (Diclofenac) were synthesized by using $POCl_3$ as a cyclodehydrating agent under microwave effect. The synthesized compounds were purified and characterized by suitable chromatographic and spectroscopic techniques. The reaction conditions were optimized so as to achieve maximum yield. Optimizing the various parameters of the microwave helped to attain a greener approach towards the synthesis of the tilted oxadiazole compounds. Factorial design used for the optimization of the synthesized compounds. The results obtained through the software confirmed that the optimum condition for attaining maximum yield by performing the microwave assisted synthesis at microwave power of 560 watts for time of 83 minutes.



(4a-4g)

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Poster Presentations

Cultivation of some important medicinal important plants and their Novel synthesis of 4-amino-2-hydroxymethyl-1-butanol and its purine analogues

Vascuri Janardhana Rao[1,2], V. Ravinder Reddy[1], Kagga Mukkanti[2], N.A.Vekariya[1]
[1]Chemical Research and Development Department, Aurobindo Pharma Ltd., 313, Bachupally, Hyderabad - 500090, Andhra Pradesh, India.
[2]Department of Chemistry, Jawaharlal Nehru Technological University, Kukatpally, Hyderabad - 500085, Andhra Pradesh, India.

ABSTRACT

A new synthetic method for the preparation of 4-amino-2-hydroxymethyl-1-butanol (1) starting from 2-acetoxymethyl-4-methanesulfonyl-1-butylacetate (5) is described via novel intermediates 6 and 7. The compound 1 is a key intermediate in the preparation of 9-[4-Acetoxy-3-(acetoxymethyl)butyl]-2-aminopurine (Famciclovir drug substance, 2). Compound 1 is coupled with 19 to results novel intermediate *N*-(2-amino-4-chloro-6-[[4-hydroxy-3-(hydroxymethyl)-butyl]amino]pyrimidin-5-yl)formamide 4. This is further converted in to purin analogue (Famciclovir) through Dechlorination, cyclisation and acetylation. Our present work describes the novel synthesis of Famciclovir drug substance (2) and 4-amino-2-hydroxymethyl-1-butanol (1).

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Thermal profile and decomposition kinetics of some synthesized 1,5-benzodiazepines

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ABSTRACT

Thermal analysis of some 1,5-benzodiazepines derived from quinoline chalcones, have been carried out by TG and DSC technique. TG data of decomposition have been analysed for the kinetic parameters using Freeman-Carroll method. From the observed curves, various kinetic parameters such as order of degradation (n), energy of activation (E), frequency factor (A) and entropy change (?S) have been evaluated. Further, thermal stability of benzodiazepines have been determined, which is found to depend on the type of substituent present in the compounds.

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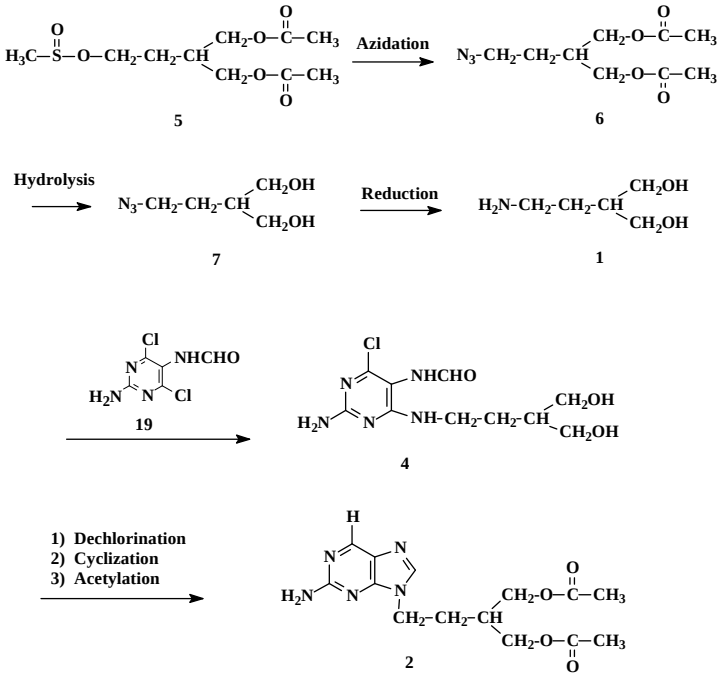
Poster Presentations

Novel synthesis of 4-amino-2-hydroxymethyl-1-butanol and its purine analogues

Vascuri Janardhana Rao[1,2], V. Ravinder Reddy[1], Kagga Mukkanti[2], N.A.Vekariya[1]
[1]Chemical Research and Development Department, Aurobindo Pharma Ltd., 313, Bachupally, Hyderabad - 500090, Andhra Pradesh, India.
[2]Department of Chemistry, Jawaharlal Nehru Technological University, Kukatpally, Hyderabad - 500085, Andhra Pradesh, India.

ABSTRACT

A new synthetic method for the preparation of 4-amino-2-hydroxymethyl-1-butanol (1) starting from 2-acetoxymethyl-4-methanesulfonyl-1-butylacetate (5) is described via novel intermediates 6 and 7. The compound 1 is a key intermediate in the preparation of 9-[4-Acetoxy-3-(acetoxymethyl)butyl]-2-aminopurine (Famciclovir drug substance, 2). Compound 1 is coupled with 19 to results novel intermediate *N*-(2-amino-4-chloro-6-[[4-hydroxy-3-(hydroxymethyl)-butyl]amino]pyrimidin-5-yl)formamide 4. This is further converted in to purin analogue (Famciclovir) through Dechlorination, cyclisation and acetylation. Our present work describes the novel synthesis of Famciclovir drug substance (2) and 4-amino-2-hydroxymethyl-1-butanol (1).



PP - 221

Poster Presentations

Mesomorphic properties of a new homologous series: 4-(4'-n-alkoxy-benzoyloxy)-3-methoxyphenyl azo-4''-chlorobenzenes

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ABSTRACT

A homologous series with carboxy (-COO-) and azo (-N=N-) as central groups have been synthesized by treating 4-n-alkoxy benzoyl chloride with 4-Hydroxy-3-methoxy phenyl azo-4'-chlorobenzene. The first and second member of the series are non-mesomorphic. The nematic property is exhibited by the propyl to hexadecyl derivatives. Polymesomorphism commences from Butyl derivative of the series enantiotropically. The mesogenic properties of the present series are compared with those of other structurally similar mesogenic series. Odd –even effect is observed for smectic- nematic and nematic-isotropic transition curve behaving in normal manner. Texture of nematic mesophaseis of threded type and that of smectic mesophase is focal conic fan shaped of the type Smectic-A or Smectic-C as determined by missibility method. analytical data support the structures of molecules.

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PP - 222

Poster Presentations

Synthesis of some quinoline derivatives clubbed with oxindole (2-Chloroquinoline-3-yl-methylene-indolin-2-ones)

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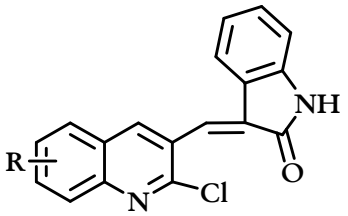
Department of Chemistry (DST-FIST & UGC-SAP Funded), & National Facility for Drug Discovery Through New Chemical Entities Development and Instrumentation Support to Small Pharma Enterprises, Saurashtra University, Rajkot-360 005.

ABSTRACT

The quinoline is widely used moiety which is found in various antibiotics, antimalarial and anticancer, such as Quinoline, chloroquine, mefloquine, hydroxyquine etc. Oxindole are endogenous compounds found in mammalian body fluids and tissues that have shown an extensive range of biological effects, including antibacterial, antifungal, anticonvulsant and antiviral activity. So keeping in view of various biodynamic activities of substituted quinoline and oxindole the synthesis of 2-Chloroquinoline-3yl-methylene-indolin-2-ones derivatives have been undertaken by the condensation of different substituted quinoline aldehyde and oxindoles. Newly synthesized compounds were confirmed by ^{1}H NMR, ^{13}C NMR, Mass and IR spectral analysis.



2-Chloroquinoline-3-yl-methylene-indolin-2-ones
(10 examples)

Where,
R = 6-CH_3, 7-CH_3, 6- OCH_3, 7- OCH_3, , 8- OCH_3, 6-NO_2, 6-Cl, 7-Cl, F, H

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Poster Presentations

Synthesis of 3-substitued indoles and evaluation of their Src kinase inhibition and antibacterial activity

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ABSTRACT

Compounds with indole nucleus are important scaffold in drug discovery. They have been shown to possess anti-cancer, kinase inhibition, antibacterial, CB2 receptors, and tubulin inhibition. Multicomponent reactions have been playing a powerful role in preparation of diverse array of compounds in one step and high yields. We have developed a novel method for synthesis of 3-substituted indoles by one-pot condensation of aldehyde, amines and indole catalyzed by $Yb(OTf)_3$ supported on silica under solvent free condition. A series of 21 compounds were synthesized by varying amine and aldehyde in 51-88 % yield. All the synthesized compounds were evaluated for Src kinase inhibition and antibacterial activities. They showed moderate inhibition of Src kinase and antibacterial activity. Details of experimental procedure and biological activities will be presented in poster.

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Poster Presentations

Ionic liquid supported synthesis of sulfonamides and carboxamides

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ABSTRACT

For past several years, solid phase synthesis has been utilized to generate large molecular libraries of small organic molecules for the discovery of active compounds in pharmaceutical research. In spite of the success of solid phase approaches for the generation of large libraries in combinatorial or parallel organic synthesis they are associated with several disadvantages such a lower loading, difficulty in characterization of intermediates and prolonged validation-time, inability to effect compound purification prior to final cleavage from the solid support, use of large excesses of reagents and difficulty and high cost of synthesis of compounds in adequate quantities for biological evaluation. Consequently, attention has increasingly turned to the identification of alternative solution-phase approaches that do not suffer from these limitations. In recent years, ionic liquid supported synthesis has aroused great interest as alternative solution-phase approach.[1] In continuation of our interest ion application of ionic liquids in organic synthesis[2] we have developed ionic liquid supported reagent for the synthesis of sulfonamide and carboxamide. A series of sulfonamides and amides were synthesized by the reaction of sulfonyl chlorides and acid chlorides, respectively to the ionic liquid supported amines followed by cleavage using trifluoroacetic acid/TEA/water. The supported reagent has been used to introduce diversity in sulfonamides through Suzuki and Heck reaction. The advantage of the protocol over solid phase synthesis is homogeneous reaction medium, high loading, easy separation of products and characterization of intermediates. The details of experimental procedure will be presented.

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PP - 225

Poster Presentations

Synthesis of novel indolyl-1,2,4-triazoles as potent and selective anticancer agents

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ABSTRACT

Indolyl heterocycles play vital role in the development of novel anti-cancer agents such as naturally occurring Vinca alkaloids vincristine and vinblastine with a continuing interest for future anticancer therapy [1, 2]. The 5-(3'-Indolyl)oxazoles, Labradorin 1 and 2 were found to be potential inhibitors of NCI-H460 human lung cancer cell line with GI_{50} values 9.8 and 9.6 μg / mL, respectively [3]. Similarly, bis(indole)alkaloids such as Topsentine, Nortopsentine and their synthetic analogues are well proven anticancer agents. Cytotoxicity of these indolyl heterocycles was explained via their interaction with microtubule assembly either by inhibition of tubulin polymerization or by blocking microtubule disassembly. Anticancer activities of indolylazoles were further improved by introduction of different heterocycles at C-3 position of indole nucleus. Our earlier findings include the discovery of 4-(3'-indolyl)oxazoles, indolyl-1,3,4-oxadiazoles and indoly-1,3,4-thiadiazoles as good anticancer agents [4-6]. In continuation to our work to find better anticancer agents, we have synthesized a diverse series of indolyl-1,2,4-triazoles (fig.1) from the reaction of indole-3-carbonitrile with appropriate acid hydrazides in presence of potassium carbonate. Synthesized compounds were evaluated for their cytotoxicity against human cancer cell lines. Details of this synthetic protocol and anti-cancer activity will be discussed in the presentation.

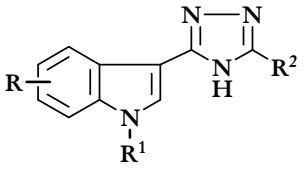

Figure 1

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Poster Presentations

Synthesis and photophysical studies of novel porphyrin thiazoles

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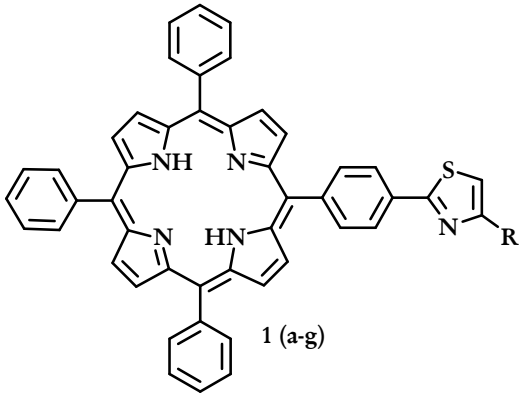
ABSTRACT

Porphyrins are tetrapyrrolic heterocyclic molecules which play important role in many biological processes such as light energy conversion, oxygen transport, metabolism and catalysis [1]. Biological effects of porphyrins largely depend on their physicochemical properties, which in turn lead to important changes in their photophysical behavior [2,3]. The presence of a conjugated double bond system in the tetrapyrrole nucleus is the structural feature responsible for the strong characteristic absorption and fluorescence [4,5]. The photochemical properties of porphyrins are largely dependent on the nature of substituents and can be tuned appropriately by varying type of metal in the porphyrin cavity or modification at β-pyrrolic and peripheral positions [6,7]. As a result, functional group interconversion and synthetic transformations related to porphyrin chemistry are continuously being explored and improved [8,9]. In literature there are various methods available for the synthesis of porphyrins molecules [8,9], however methods for structural modification of porphyrin molecules are rare. Thus, development of facile, efficient and versatile synthetic strategy to functionalize porphyrin molecules with appended heterocycles is of a high interest to broaden their scope of utilizations. In continuation of our efforts towards development of novel porphyrin molecules for anti cancer agents [10], we have synthesized porphyrin appended thiazoles (fig. 1) and studied their fluorescence properties. The details of the fluorescence studies and synthesis will be presented at the conference.



1 (a-g)

Figure 1

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Poster Presentations

Study of new homologous series of azoester mesogens: p-(p'-n-alkoxybenzoyloxy)-m-methylphenylazo-p"-methoxybenzene

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ABSTRACT

A new homologous series of azoester mesogens: p-(p'-n-alkoxybenzoyloxy)-m-meyhyl phenylazo-p''-methoxybenzenes has been synthesized with a view to understand the relation between liquid crystal preparation and molecular structure. Transition temperatures of the members of the homologous series are observed under Leits Labourlux 12 POL-polarizing microscope with heating stage. The homologues of the series show variation in textures and transition temperatures. Mesomorphism commences from the very first homologue of the series. All the members of the series exhibit enantiotropic mesomorphism except third member which exhibit monotropic-nematic behavior. Smectic mesophase commences from the dodecyl homologue of the series. Dodecyl homologue of the series exhibit polymesomorphism i.e. smectic and nematic phase are present, one after another. The series is of high melting type with considerable mesomorphic range. The thermal stabilities and mesomorphic properties of the series have been compared with other structurally similar homologous series. Texture of the nematic mesophase is of threaded type and that of smectic mesophase is, focal conical fan shaped of type- A for dodecyl and tetradecyl homologue and smectic-C for hexadecyl homologue as determined by miscibility method. Analytical data support the structure of molecules.

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PP -228

Poster Presentations

3, 7-Disubstituted coumarin: an efficient fluorescent probe for protein bioconjugation

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ABSTRACT

Coumarins and its derivatives have wide application in the field of medicine due its various biological activities. They are also used as probe molecules for biomedical diagnostics and bioinformatics. To study the interaction of organic fluorophores with biological system is interesting for biologists and chemists. These interactions are useful in clinical diagnosis and theranostics. These principles are also of importance in environmental monitoring, online monitoring of bioprocesses, and immunology-based sensing. Since radiological techniques are considered harmful fluorescent molecules are gaining importance as molecular probes. Organic fluorophores however suffer from less biocompatibility, lower fluorescence lifetime, photophysical and photochemical stability and low fluorescent quantum yield in the biological microenvironment[1]. For these study novel fluorescent fluorophores which have high fluorescent lifetime, high photo stability, and appreciably higher fluorescence quantum yield are being developed.

In the present study various novel fluorescent molecules which can function as molecular probes on bioconjugation are designed and synthesized from substituted coumarins. Interaction of synthesized fluorophores with protein bovine serub albumin is studied. Photophysical properties of fluorescent molecules as well as their bioconjugates like absorption emission characteristics and fluorescent quantum yield are reported. Proposed molecule is shown in figure.

The novel fluorescent molecules which function as recognition elements in the probes are confirmed by FT-IR, ^{1}H NMR and mass spectral analysis. Photo–physical and thermal studies were done by UV-Vis. Spectrofluorometer and thermo gravimetric analysis. The bioconjugation was carried our using the protein, bovine serum albumin.

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Poster Presentations

Synthesis of pyrazolo[3,4-*d*]pyrimidinophanes for ^{1}H and x-ray crystallographic studies

Tejprakash Singh,[a] A. Ansari,[a] R. Kant,[b] P. R. Maulik,[b] K. Avasthi,[a]*
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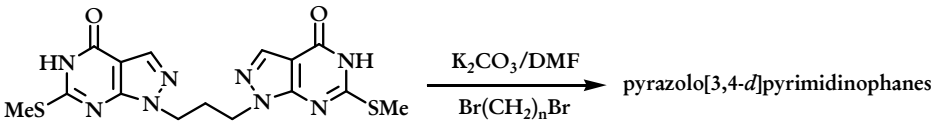
ABSTRACT

Cyclophanes are chemical species in which one or more aromatic unit are interbridged by an aliphatic chain in such a fashion to form a cyclic garland of aromatic core and aliphatic linker. Cyclophanes are good models for studying "host-guest interactions," "molecular recognition" and "transannular π–π interaction". Cyclophanes were initially studied by Cram and Steinberg in 1951.[1] Systematic studies on purinophanes were reported by Seyama *et. al*. in 1988.[2] Generally, the synthesis of cyclophanes involves the transformation of monobridged compound into di-bridged one, in which the yield is often poor due to competing intermolecular reaction forming oligomers. Use of pre-organized mono-linker starting material, also called protophanes, may increase yield of cyclophanes considerably.[3] Thus, reaction of monobridged compound (1), assumed to be folded, due to the fact that many related compounds show folded conformation in solid state due to intramolecular π–π interaction,[4] was studied for the synthesis of pyrimidinophanes (2).



(1) (2)

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Poster Presentations

In vitro DNA damage and hepatoprotective activity of hydroethanolic extracts of *Ficus glomerata* fruit

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ABSTRACT

Several types of reactive oxygen species are generated in the body as a result of metabolic reactions in the form of free radicals or non-radicals. They attack macromolecules including protein, DNA and lipid etc. causing cellular/tissue damage. To counter their effect, the body is endowed with another category of compounds called antioxidants. These antioxidants are produced either endogenously or received from exogenous sources and include enzymes like superoxide dismutase, catalase, glutathione peroxidase and glutathione reductase. In a healthy body, pro-oxidants and antioxidants maintain a ratio and a shift in this ratio towards prooxidants gives rise to oxidative stress. This oxidative stress may be either mild or severe cause of several diseases such as cardiovascular diseases, neurological diseases, malignancies, renal diseases, diabetes, inflammatory problems, skin diseases, ageing, respiratory diseases, liver diseases and different types of viral infections. Antioxidant properties elicited by the plant species have a full range of perspective applications in human healthcare. The aim of this study was to see the effects of hydroethanolic (1:1) extracts of fruit on antioxidant system, *in vitro* DNA damage and hepatoprotective activity. The antioxidant activity was estimated on the basis of total phenolic content (TPC), DPPH radical scavenging and reducing power activity. The ripened fruit extract showed highest antioxidant activity. The extracts also showed dose dependent *in vitro* DNA damage protection against UV light and significant hepatoprotective properties against acetaminophen toxicity.

DNA damage and hepatoprotective activity. The antioxidant activity was estimated on the basis of total phenolic content (TPC), DPPH radical scavenging and reducing power activity. The ripened fruit extract showed highest antioxidant activity. The extracts also showed dose dependent *in vitro* DNA damage protection against UV light and significant hepatoprotective properties against acetaminophen toxicity.

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Poster Presentations

Effect of oxidizing as well as reducing agents on the reduction of molybdenum (VI) in presence of alizarin red using differential pulse polarography

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ABSTRACT

In this study the effect of reduction of Molybdenum with Alizarin red in the presence of different oxidizing agents such as KNO_3, $NaNO_3$, $KClO_4$, and reducing agent such as Hydrazine, KCl and NaCl were employed. The method proposes that, $NaNO_3$ is the best oxidizing agent and NaCl is the best reducing agent for the reduction of Molybdenum using Differential Pulse Polarography. The polarograms were recorded at pH 2.0 (HCl buffer) and also for the unbuffered and unadjusted condition for both oxidizing as well as reducing agent. The good current concentration linearity was observed in these conditions.

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Studies on newly synthesized benzimidazoles and benzothiazoles

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ABSTRACT

Benzimidazoles and benzothiazoles were synthesized in excellent yield by 1,2-phenylenediamine and 2-aminothiophenol respectively with pyrazol aldehydes as a starting material using hydrogen peroxide and ceric ammonium nitrate (CAN) as a catalyst. All the newly synthesized compounds were characterized by spectroscopic studies such as ^1H NMR, IR and Mass spectroscopy.

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Artemisinin and its derivatives as inhibitors of antioxidant system of *Plasmodium yoelii*.

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ABSTRACT

Malaria is amongst the most prevalent parasitic diseases in the tropics. 95% of the malarial cases are due to *P. falciparum* and *P. vivax.* The antimalarials viz., 4-aminoquinolines, 8-aminoquinolines, amino alcohols and antifolates have been used in the control and treatment of the disease, however due to increasing incidences of drug resistance in recent years development of new antimalarials is needed. Quinine resistance have been reported in *P. falciparum* from Brazil and South East Asia and Artemisinin is being used for treating such antimalarial resistance parasites. Oxidative stress is an important mechanism for the destruction of malarial and other intracellular parasites. The intra erythrocytic stages of malarial parasite encounter reactive oxygen species produced either by erythrocytes or host immune cells. In order to prevent oxidative damage, the parasite would both commandeer host enzymes and reduced its own antioxidant enzymes. The erythrocytes itself have potent antioxidant defences to counteract production of ROS by oxidation of haemoglobin of methaemoglobin. The malarial parasite contained antioxidant enzymes viz., SOD catalase and GPX in different developmental stages. The effect of Artemisinin and its derivative was studied in rodent malarial parasite *P. yoelii.* The Artemisinin and its derivative were found to inhibit the antioxidant defence enzymes of infected erythrocytes. The antimalarials affected the antioxidant enzymes of the *P. yoelii* to different extent. Incubation of Artemisinin and its derivative with infected blood for one hour also exerted significant inhibitory effect on the antioxidant system of the erythrocyte as well as parasite. Artemisinin and its derivatives appear to significantly inhibit the antioxidant system of the malarial parasite.

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Role and future of chemistry and biology in current century

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ABSTRACT

In this new pragmatic century all branches of sciences are interwoven,in fact chemistry and biology has a tremendous role to play., .Chemistry has been continously and rapidly developing, it has a major responsibility to sustain the environment of the earth and we must find ways for humans and nature to co exist indefinetly, that is in modern terminology to achieve sustainable society.Extensive high level research in the chemical and biological sciences together have strongly influenced the promotion of their interfacial sciences ,including biological chemistry,biotechnology,nanosciences and nanotechnology. Rapid increases in human population, overcrowding, environmental degradation and rapid transport have all enhanced the spread of existing infectious diseases as well as the threat of newly emerging infections. .Hence the advances in diverse areas of chemistry and biology should be used to discover therapeutics for all types of diseases. Finally the paper highlights the researches of how natural product chemistry is one way to examine biological phenomenon such as diseases/drug action, synthesis of small molecule libraries and bioprobes, that can be used as chemical tools to probe interesting biological activities. In the 21st century it is expected that molecular chemistry and supramolecular chemistry will develop in parallel ,it will deepen not only our understanding of living organism but also our research in the field of molecular chemistry. Future of chemistry and biology lies in synthethic biology (development & use of "biobricks" to develop first artificial organism), personal genomics, nootropics, cosmoceuticals in which chemoinformatics and bioinformatics will play a vital role. To conclude, it is certain that both chemistry as well as biology in the 21st century must keep a good balance with nature so that we can lead a affordable, healthy and sustainable life.

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Poster Presentations

Synthesis of 2-azetidinones as potential anti-microbial and anti-tubercular agents

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ABSTRACT

Microorganisms are the cause of many infectious diseases like pneumonia, plague, gas gangrene, wound sepsis & tuberculosis. These microorganisms were in past responsible for killing more people than any other disease. Currently used antimicrobial agents are not very useful due to resistance developed by the microbes. So there is a need to develop new antimicrobial agents. 1, 2, 4-Triazole is an important pharmacophore and have a wide range of therapeutic properties[3-6]. Azetidinones are part of antibiotics structure and are known to exhibit interesting biological activities. 2- Azetidinones are more commonly called as β-lactams. A variety of 3-chloro monocyclic β-lactams exhibit powerful anti-bacterial, anti-fungal, anti-inflammatory, anti-convulsant and anti-tubercular activities[7-10]. Azetidinones also function as enzyme inhibitors and are effective on the central nervous system. Thus a series of 3-chloro-4-(4-substituted-phenyl)-(1*H*-[1, 2, 4]-triazole-3-yl)-amine is synthesized using 3-amino-1, 2, 4- triazole as a starting material. First the Schiff's bases were synthesized from 3-amino 1, 2, 4-triazole using different aldehydes in the presence of catalytic amount of glacial acetic acid. Schiff's bases obtained were cyclized into 2-azetidinones using chloracetyl chloride and triethylamine. Compounds obtained were purified either by column chromatography or recrystallization using suitable solvents. Purified compounds were characterized by IR, Mass & ^{1}H-NMR. Compounds were evaluated for their anti-bacterial against *E. Coli* and *S.aureus* & antifungal activity against *A. niger* and *C .albicans*. Anti-tubercular activity was also tested against *M. tuberculosis*. Most of the compounds have shown moderate to good activity.

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Poster Presentations

Hepatoprotective activity of *Jatropha curcas* L. against ethanol induced liver injury in rats

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ABSTRACT

Jatropha curcas L. (Euphorbiaceae) is indigenous to Mexico and Central America and commonly known as wild castor in India[1]. The phytochemical screening of leaf of this plant showed presence of alkaloids, steroids, flavonoids, saponins, terpenoids, carbohydrates, tannins and the leaf is reported to be medicinally important in traditional system of medicine [2, 3]. The aim of this work is to study hepatoprotective effect of hydroalcoholic extract of leaf of *Jatropha curcas L.* against ethanol induced hepatic damage [4]. The acute toxicity studies of the extract showed no signs of toxicity up to dose level of 2000 mg/kg given orally [5]. The oral administration of hydroalcoholic extract of *J.curcas* (250 mg/kg/day and 500 mg/kg/day) for 7 days decreased the level of biochemical markers of liver injury like ALT and lipid peroxidation whereas level of GSH was found to be increased. Further, the histopathological studies were also carried out. All the results obtained were compared with reference drug silymarin, from which it can be concluded that *J.curcas* possesses significant hepatoprotective activity.

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Poster Presentations

Synthesis and assessment of analgesic activity of novel 2, 5-disubstituted-1, 3, 4-oxadiazole

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ABSTRACT

Over the past two decades and still on, molecular biologists are leading a quiet revolution in understanding pain, exploring its pathophysiology and leading to new drug development and design. Pain is the most common complaint in the medical field; the arsenal of effective and safe analgesics is still relatively small. Thus, the search for compounds that can effectively treat painful states without induction of side effects remains a major challenge in biomedical research. 1, 3, 4-Oxadiazoles are well known compounds which exhibit diversified biological activities and are the bio-isosteres of amides and esters. Due to increased hydrolytic and metabolic stabilities of the oxadiazole ring, improved pharmacokinetic and in vivo performance is often observed. 1, 3, 4-Oxadiazoles were synthesized by reacting substituted anilines with ethylchloroacetate in presence of triethylamine and refluxing these esters with hydrazine hydrate in methanol yielding various hydrazide derivatives. Finally, the target molecule 2, 5-disubstituted-1, 3, 4-oxadiazoles were synthesized by refluxing the hydrazides with substituted aldehydes. Structure elucidation of the synthesized compounds was established by IR, NMR and mass spectroscopic techniques. The synthesized derivatives were evaluated for their in vivo analgesic activity by acetic acid induced writhing method in mice at two dose levels 25 and 50 mg/kg of body weight. Diclofenac sodium was used as a standard drug at a same dose levels. All the synthesized compounds exhibited antinociceptive activity among which 3-chloro-N-((5-(3,4-dimethoxyphenyl)-1,3,4-oxadiazole-2-yl)methyl)-4-fluoroaniline and N-((5-(3,4-dimethoxyphenyl)-1,3,4-oxadiazole-2-yl)methyl)-4-methylaniline were found to exhibit highest degree of analgesic activity. These studies would provide insights into the design of better molecules in future.

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Poster Presentations

Receptor-ligand based pharmacophore modeling of checkpoint kinase 1 (chk-1) inhibitors

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ABSTRACT

Checkpoint kinase 1 (ChK-1) is a serine-threonine kinase that plays an important role in the DNA damage response, in the G2/M cell cycle phase. Inhibition of ChK-1 kinase by small molecules is of great therapeutic interest for oncology and in understanding the cellular regulation of the G2/M checkpoint {Graves et al.}. We have developed a pharmacophore hypothesis for known ChK-1 inhibitors. The pharmacophore hypotheses were developed using two known techniques viz. the receptor-ligand pharmacophore (receptor dependent) and the common feature pharmacophore (receptor independent) {Guner et al.}. The receptor-ligand pharmacophore was developed using a single bound ligand conformation while the common feature pharmacophore was built from the pharmacophoric elements present in the set of diverse structures. In addition, the effect of alternate conformations was also tested in the common feature pharmacophore case. All the generated hypotheses were analyzed and the study revealed that the best and ideal hypothesis should have four chemical features viz. two hydrophobic and two H-bond acceptors. These chemical features were found consistent among the different models across the classes. This was substantiated by the cluster analysis of the different pharmacophore hypothesis which showed an RMSD value in the range of 0.07-0.098. The models were externally validated using a decoy dataset premixed with a set of known actives. These results might provide guidance for the rational design of novel potent and selective ChK-1 inhibitors.

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Poster Presentations

An activity model for novel antidepressants that interact with the serotonin transporter protein (SERT)

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ABSTRACT

Serotonin is one of the primary neurotransmitters involved in the depression pathophysiology. The molecules that enhance the level of serotonin through blockade of serotonin re-uptake or by inhibition of serotonin metabolism are effective antidepressants. A set of new molecular entities (NME-24, NME-16, NME-5 and NME-2) have been synthesized which are active in animal models of behavioral despair and are hypothesized to work by modulating the serotonin neurotransmission {Kessar et al.}. The present study attempts to correlate via molecular modeling the binding of these new NMEs to the serotonin transporter protein (SERT) with the behavioral pattern observed in the mouse forced swim test (FST) model which is an animal model for depression. Initially a homology model of SERT was built using the X-ray crystal structure of Leucine Transporter (LeuT) as the template {Jorgensen et al.}. The NMEs were docked into the active site of the SERT to identify the putative binding orientations. 3D-QSAR models based on the CoRIA formalism {Datar et al.} were generated from the experimental data and docking scores for some INDs of SERT inhibitors. The CoRIA models shed light on the salient features necessary for effective binding of NMEs to the serotonin transporter and can also predict the pKd values. A significant correlation has been observed between the anti-immobility effect demonstrated in the mouse FST study and the binding energies obtained from the docking study. The pKd values from the CoRIA models and the inhibition values from the mouse FST show a similar trend, ranking molecules as: NME-24 > (NME-16 = NME-5) > NME-2 > venlafaxine.

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Poster Presentations

Synthesis of amino acid conjugates of 4-Aminoquinolines as potent antimalarial agent

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ABSTRACT

Malaria is one of the most widespread tropical parasitic diseases, caused by the protozoa of the genus plasmodium and transmitted by the female Anopheles mosquito. Today, over 40% of the world's population is at risk from malaria estimated to affect 300-500 million people world wide and it is responsible for about 2 million deaths each year1,2. It is endemic in tropical regions including India. Malaria is caused by four different types of parasites, Plasmodium falciparum, P. malariae, P. vivax and P. ovale. Among these, P. falciparum is the most fatal affecting all ages with multiple-systemic complications like unarousable coma, severe anemia, repeated seizures and hepatopathy. In India especially Northeastern regions are one of the hot spots for malaria transmission. Focal outbreaks of malaria are of common occurrence especially in forest-fringed villages of Assam, bordering Arunachal Pradesh3.Orissa alone contributes to more than 40% of falciparum deaths in India, south Orissa is a known hyper-endemic area of the state4. The developments of Chloroquine resistant strains are further complicating the situation. In the quest of superior CQ analogs which could be active against resistant strains, a number of new molecules were synthesized and tested. These studies suggested that 7-chloro-4-aminoquinoline nucleus is most suitable for antimalarial activity, particularly, inhibition of hematin formation and accumulation of the drug at the target site 4, 5. But modifications inside the chain viz. carbon chain length and basicitity of nitrogen in chain of CQ have significant impact on activity 6. Considering these two facts we have designed molecules where amino acids are condensed in side chain. Amino acids impart a chiral center to the molecule and provide opportunity to study a variety of lipophilic moieties in the side chain. Coupling of amino acid with various amines gave different amides which were fused finally with DCQ to afford final compounds. These modifications have been done according to bioisosteric concepts. Details of synthetic procedure and biological activities of these compounds will be discussed in detail.

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Poster Presentations

Synthesis and biological evaluation of thiazolo [3,2-a] pyrimidine derivatives as a new type of potential antimicrobial agents

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ABSTRACT

A series of 2-(ary)-4-(4'-methoxyphenyl) – N - (3,4-di methylphenyl) - 3,5 – dihydro – 7 -methyl – 3 – oxo - 5-phenyl-2H -thiazolo [3,2-a] pyrimidine - 6 –carboxamide compounds were synthesized under reflux condition by a simple one pot condensation reaction of 4 – [(p-methoxyphenyl)-5 - (3,4 – dimethyl) –phenyl amino carbonyl] – 6 – phenyl - 1,4 –dihydro pyrimidine -2(1H) –thiones and monochloro acetic acid, glacial acetic acid, acetic anhydride and different aromatic aldehydes in the presence of sodium acetate, where, thiopyrimidine derivatives were prepared by three component Biginelli reaction in presence of hydrochloric acid as a catalyst. The yield of both type of compounds thiopyrimidine derivatives and thiazolo pyrimidine derivatives following recrystallisation from proper solvent were of the order 55 -80%. All newly synthesized compounds were characterized by elemental analysis, IR, 1H-NMR, and Mass spectral analysis and purity of each compounds were checked by TLC using precoated silica gel plate. The synthesized compounds have been screened for their antimicrobial activies against various gram positive and gram negative bacteria and fungi. Where MIC of each compound were also determined.

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Poster Presentations

An efficient synthesis of some novel pyrazolines, isoxazoles, and their anti-microbial and anti-tubercular activity

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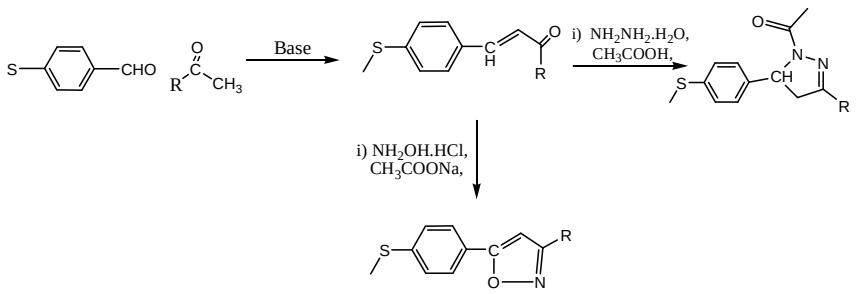
ABSTRACT

An efficient and convenient synthesis of various novel pyrazolines and isoxazoles derivatives has been described by the cyclocondensation reaction of 3-(p-methylthiophenyl)-1-aryl-2-propene-1-one with binucleophiles such as; hydrazine hydrate and hydroxyl amine hydrochloride. The newly synthesized compounds were evaluated for their *in vitro* antimicrobial and anti- tuberculosis activity. Among them few compounds were exhibited potent antimicrobial activity against gram +*ve* and gram –*ve* strains.



Where R = Ar. And Base :NaOH/KOH

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Poster Presentations

Synthesis of biologically active steroidal derivatives

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ABSTRACT

Recently there has been a resurgence of interest in the chemistry and biochemistry of steroids, which have largely been overshadowed for the past few years. These molecules have been found to play an important role in many molecular processes.

We the objective of synthesizing model compounds for use in biological studies and as a part of our programme devoted to the synthesis of some steroidal derivative, we have adopted some novel one pot synthetic methods for the introduction of various groups into the steroid nucleus. Attempts have been made to synthesize various C-3 substituted derivatives of diosgenin by treating with different aromatic and aliphatic acids using different solvent mediums in presence of DCC.

The spiroketal side chain of the sapogenin-diosgenin was cleaved to give novel pregnane moiety, which was treated with some novel aliphatic as well as aromatic halogenated amines in presence of Lewis acid catalyst, yielding some novel biologically active pregnane derivatives.

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Increased chemoprevantive activity of indol-3-carbinol (I3C) by some life essential metals Fe, Zn, and Cu (II)

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ABSTRACT

The formation of complexes among the Indol-3-carbinol, Fe,Zn,Cu (II) was studied in aqueous media with in the pH 5.7±0.1 by means of polarography, amperometry and spectrophotometry. The polarogram of acidic media indicated that a chemical reaction has taken place between and Fe, Zn,Cu (II), shows that formation of complexes. The Indol-3-carbinol produce a well defines direct current polarogram and differential pulse polarogram in 0.1 M ammonium tartrate (supporting electrolyte) at pH 5.5±0.1. The stoichiometry of Fe,Zn,Cu (II) – I3C complex is 1: 1. Anticancer studies on the drug and its metal complex have been performed against Hella cancer cell line (*In Vitro*). The observed results revealed the complex to be more potent in anticancer activity as compared to the parent drug.

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Poster Presentations

Hypolipidemic, hypoglycemic and anti oxidant activity of flower extracts from *Allamanda violacea*

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ABSTRACT

A. violacea (purple allamanda, violet allamanda, syn A. blanchetti) is an ornamental plant of Allamanda genus in the Apocyanaceae family. The ethanolic extract of the roots, leaves and stems of this plant have previously been shown to posses cytostatic and cytotoxic activity. Aqueous extract of Allamanda violacea flowers showed significant anti-hyperlipidemic, antiglycemic and anti-oxidant activity. Aqueous extract was fractionated into Pet ether, ether, chloroform, chloroform-methanol (4:1) and chloroform-methanol (3:2) fractions. These extracts were subjected to phytochemical tests for the detection of carbohydrates and/ or glycosides, tannins, flavonoids, sterols and/or terpenes. All the extracts responded positively to the Feigel , Vanillin perchloric acid test (for the presence of 2-deoxy and 6-deoxy sugars) and NaOH tests (for flavonoids) whereas pet ether, ether and chloroform extracts gave positive Libermann Burchardt test (for sterol and/or terpenes) and Liquid ammonia test (for flavones), indicating the presence of flavones/sterols/ terpenes in their free state or in form of their glycosides.

The lipid lowering activity of these five fractions was evaluated in two models viz, triton WR-1339 induced hyperlipimea in rats as well as fructose rich high fat diet. Activity (*in vivo*) was found to be concentrated in ether and chloroform-soluble fractions. The antioxidant activity of these five fractions was assessed *in vitro*. These fractions when tested against generation of oxygen free radicals at concentrations (100-200 ìg/ml), counteracted the formation of superoxide anions O_2^- and hydroxyl radical (·OH) in non enzymic test systems. Ether and chloroform fraction also showed potent antioxidant activity in this test system while other fractions showed mild antioxidant activity. The hypoglycemic activity of these extracts was also evaluated.

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Poster Presentations

Synthesis of some 1H-2,3-dihydrocyclopenta [1',2';5,6] pyrido[3,2-*c*] coumarins; 1,2,3,4-tetrahydroquino[3,2-*c*]coumarins and 5,6-dihydro-14-aza-benzopyrano[4,3-*b*]phenanthrene-8(H)-ones

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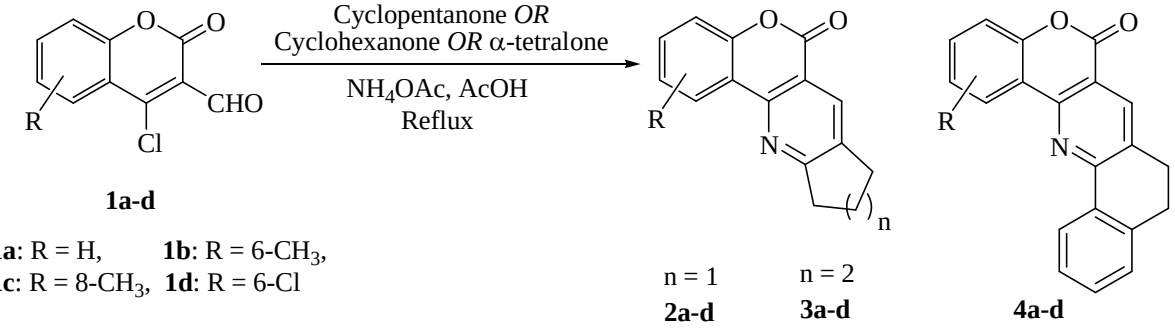
ABSTRACT

Coumarins(2H-1-benzopyran-2-ones) are best known aromatic lactones isolated from variety of plant extracts. Due to their diverse biological activities viz. anticoagulant, antibacterial and antifungal, many natural, semi synthetic and synthetic coumarins possess a prominent place in drug research. In this direction, several biological activities have been claimed for compounds comprising both coumarins and coumarins fused to pyridine ring. Coumarins fused with pyridine have strong evidence to possess antiallergic, anticoagulant and antidiabetic activities. In continuation of our interest in synthesizing various pyrido[3,2-*c*]coumarins and modifying the pyridine moiety, herein we report the synthesis of some 1H-2,3-dihydrocyclopenta [1',2':5,6]pyrido[3,2-*c*]coumarins; 1,2,3,4-tetrahydroquino[3,2-*c*]coumarins and 5,6-dihydro-14-aza-1-benzopyrano[4,3-*b*]phenanthren-8(H)-ones.

The title compounds(2a-d, 3a-d and 4a-d) have been synthesized by reacting various 4-chloro-3-formyl coumarins(1a-d) with cyclopentanone, cyclohexanone and á−tetralone in the presence of ammonium acetate and acetic acid. All the synthesized compounds were characterized by analytical and spectral data and also screened for antimicrobial activity.



1a-d

1a: R = H, **1b**: R = 6-CH_3,
1c: R = 8-CH_3, **1d**: R = 6-Cl

n = 1 **2a-d**

n = 2 **3a-d**

4a-d

PP -247

Poster Presentations

Synthesis and characterization of 4-thiazolidinones from 5-ethyl pyridin-2-ehanol: their antibacterial, antifungal and antimycobacterial activity

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ABSTRACT

Thiazolidinone 5a-o derivatives were prepared from the reaction of Schiff base and thioglycolic acid in presence of $ZnCl_2$. The structures were assigned on the basis of elemental analysis, IR, ^1H NMR ^{13}C NMR and Mass spectral data. All the compounds were screened against different strains of bacteria and fungi. Compounds 4e, 4n, 4m, 4o, 5e, 5f, 5j and 5m possessed very good activity against bacterial and fungal species. These active compounds impelled us to study their antitubercular activity. Compounds 4n and 4e showed MIC 25 μg/ml and 62.5 μg/ml respectively, whereas compound 5m displayed MIC 25 μg/ml showed better antitubercular activity against *M. tuberculosis* compared with rifampicin.

PP -248

Biosorption of Pb(II) ions from aqueous solutions by Pre-treated biomass of Tamarind indica fruit shell

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ABSTRACT

The adsorption of lead (II) ions from aqueous solution has been investigated on formaldehyde polymerized Tamarind indica fruit shell (FPTIFS), at room temperature. The biosorbent is characterized by FTIR. The biosorption experiments were carried out in batch system as a function of pH, contact time, adsorbent dose, temperature and initial concentration of Pb (II) ions. Biosorption was pH dependent and maximum removal of Pb (II) was obtained at 5.0. The equilibrium was established in 2 hrs. Langmuir, Freundlich, Tempkin, and Dubinin-Radushkevich adsorption isotherm models were applied to the equilibrium data. The equilibrium data are satisfactorily fitted in the order off Langmuir > Freundlich > Tempkin > Dubinin-Radushkevich. The maximum biosorption capacity was 29.9 mg g^{-1}. The kinetics of Pb (II) ions adsorption was very well described by pseudo -first order and pseudo –second order kinetic models but fitness is high with later with high R^2 values exceeding 0.999. The result of study showed that the tamarind fruit shell can be efficiently used as low cost alternative for the removal of divalent lead from industrial west water.

PP -249

Poster Presentations

Synthesis, characterization and antimicrobial activities of s-triazine derivatives

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ABSTRACT

Novel series of compounds containing 1,3,5-triazine (s-triazine) derivatives have been synthesized. The purity and characterization of all the formed compounds have been checked by physical methods (melting point, TLC, elemental analyses) and by spectral data (IR & NMR). The newly synthesized compounds have been evaluated for antimicrobial activity against variety of bacterial strains in which some of these derivatives exhibited potential antibacterial and antifungal activity.

PP -250

Synthesis of 4-thiazolidinones and 2-azetidinones from chalcone and evaluation of their antibacterial and antifungal activities

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ABSTRACT

1'(3-Hydroxy-phenyl)-3-thiophene-2-yl-propenone **1** was obtained from the reaction of heterocyclic aldehyde with substituted acetophenone. The treatment of **1** with guanidine nitrate produced 3'(2-amino-6-thiophene-2-yl-pyrimidine-4-yl)phenol **2.** The synthesis of 3-[2-(benzylidine-amine)-6-thiophene-2-yl-pyrimidine-4-yl]-phenol **3a-j** was performed by the treatment of compound **2** with the corresponding aromatic aldehydes. The reaction of **3a-j** with thioglycolic acid and thiolactic acid formed the corresponding 4-thiazolidinones **(4 & 5)** and with chloroacetylchloride it gives 2-azetidinones **6**. All the Newly synthesized compounds were characterized by IR, NMR and elemental analysis. The compounds were screened against certain bacterial and fungal strains.

PP -251

Poster Presentations

Synthesis and biological evaluation of some novel sydnone based derivatives

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ABSTRACT

A series of compounds containing sydnone based chalcone and pyrimidine derivatives were synthesized. The formed compounds have been evaluated by physical methods (melting point, TLC, elemental analysis) and by spectral data (IR & ^{1}H-NMR). The antimicrobial evaluation of newly synthesized compounds showed that some of them revealed promising antimicrobial activity.

PP -252

New methodology and new technology for chemical synthesis

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ABSTRACT

Chemical synthesis pertains to the construction of new molecules-known and unknown by application of known or conceivable reactions. An ideal synthesis should be very efficient with minimum inputs. A good synthesis should also be environment friendly releasing no wastes or minimum non toxic wastes. Starting material must be readily available. Multiple component synthesis should be preferred if sequential reaction involved in the synthesis it would be desirable if all the reactions occur in one pot without isolation and purification of the intermediates. Such processes are known as domino, cascades or tandem reactions. The atom economy should be 100% or close to it. The reaction in all synthetic routes should occur at mild conditions and high selectivity of products. The solvent or catalyst employed should not be toxic that is cleaner technology with use of super critical fluids should be employed. An analytical approach namely retro-synthetic analysis has been involved. A good chemical synthesis should be innovative ,elegant and even artistic. Biological modes of synthesis are environmentally friendly synthetic protocols with selective conversion.

PP -253

Poster Presentations

Synthesis and antimicrobial evaluation of new sydnone based quinazoline derivatives

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ABSTRACT

The highly accelerated Niementowski synthesis of quinazoline derivatives has been synthesized from anthranilic acid. Which on further Reduction, Esterification, Hydrolysis, Nitrosation and Cyclization gives sydnone based quinazoline derivatives. All the synthesized compounds have been characterized by TLC, elemental analysis and spectral techniques like IR, ^{1}H-NMR and also screened for their antimicrobial activities.

PP -254

Preparation and MIC of 5-Aryl-7-methyl-N-(2,5-dimethylphenyl)-2,3,5-trihydrothiazolo[3,2-a]pyrimidine-6-carboxamides derivatives

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ABSTRACT

Thiazolopyrimidines possess significant pharmacological importance due to various biological activities such as antidepressant, antiviral, calcium channel blockers, anticancer etc. Some new thiazolopyrimidine derivatives have been prepared by the condensation of N-(2,5-dimethylphenyl)-6-methyl-4-aryl-2-thioxo-1,2,3,4-tetrahhdropyrimidine-5-carboxamides with 1,2-dibromoethane.The constitution of all the above products have been supported by elemental analysis IR,1H NMR and Mass spectrometric analysis. Purity of all the compounds have been checked by thin layer chromatography using appropriate solvent systems. All the compounds have been evaluated for their antibacterial activity against Gram Positive bacteria and Gram Negative bacteria and they were also evaluated for antifungal activity. Their antimicrobial effect was determined in higher dilutions using Agar Dilution Method(Approved by NCCLs).The potent compound of the series was further tested for tertiary screening to find exact MIC.

PP -255

Poster Presentations

Synthesis and evaluation of chalcones of 2-(4-acetylphenylamino)pyridine-3-carbonitrile as antimicrobial agents

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ABSTRACT

Keto group of cyano pyridine moiety have been treated with various aromatic aldehydes to give corresponding chalcones. The Chalcones have been reacted with hydrazine hydrate and glc acetic acid to get corresponding novel pyrazolines, The structure of all newly synthesized compounds were confirmed by spectral analysis. The synthesized compounds were evaluated for their antimicrobial activity. All the synthesized substituted pyrazolines have show good to moderate antimicrobial activity.

PP -256

New 2,4-thiazolidinedione derivativatives containing 2-amino-6-thiocyanato benzothiazole and their antimicrobial & antiviral evaluation

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ABSTRACT

In our continuous effort to make medicinally important molecule, we present here the synthesis and *in vitro* antimicrobial and antiviral activity of new series of (E)-2-(5-substitutedbenzylidene-2,4-dioxothiazolidin-3-yl)-*N*-(6-thiocyanatobenzo[d]thiazol-2-yl)acetamides. The structures of title compounds were established by elemental, IR, ^{1}H NMR and ^{13}C NMR spectral data. All the synthesized compounds were evaluated for their antibacterial, antifungal, antitubercular and anti-HIV activities. Some of the compounds exhibited good antimicrobial activities compared to standard drugs. One of the intermediate 2-chloro-N-(6-thiocyanatobenzo[d]thiazol-2-yl)acetamide showed significant cytotoxic for MT-4 cells ($CC_{50} < 10\ \mu M$).

PP -257

Poster Presentations

Design and Synthesis of aryl piperazine-derived constrained analogs of NVP-DPP728 as DPP-IV Inhibitors

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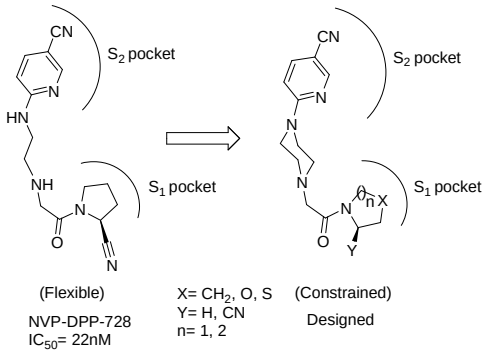
ABSTRACT

Dipeptidyl peptidase-IV (DPP-IV) inhibitors are expected to be the next major drug class for the treatment of type 2 diabetes. DPP-IV, a ubiquitous serine protease, is responsible for inactivating the incretin hormones i.e. glucagon-like peptide 1 (GLP-1) and glucose dependent insulinotropic polypeptide (GIP). These hormones play important roles in glucose homeostasis in glucose-dependent manner. Thus, a small molecule inhibitor of DPP-IV can extend the duration of action of incretins and prolong the beneficial effects of these incretin hormones. Sitagliptin (piperazine derivative), Vildagliptin and Saxagliptin are potent, orally bioavailable and highly selective small molecule DPP-4 inhibitors and have been launched in the US or EU. DPP-IV inhibitors are free from side effects such as hypoglycemia, weight gain and exhaustion of pancreatic â-cells. Several DPP-IV inhibitors are currently being evaluated in human clinical trials including Alogliptin, Dutagliptin and PF-00734200 (piperazine derivative).

Among various DPP-IV inhibitors reported so far, NVP-DPP728 is potent and slow binding inhibitor of DPP-IV [1]. In several studies, it has been found that, when NVP-DPP728 displays inhibitory activity, the [2-(5-cyanopyridyl)amino]ethyl moiety of assumes not an extended but a folded conformation (Figure-1). NVP-DPP728 analogs having a rigid conformation may show potent inhibitory activity [2]. DPP-IV inhibitors having (S)-2-cyanopyrroldine moiety at P_1 position are chemically unstable due to intramolecular cyclization between amine group and their electrophilic cyano group. On the basis of above assumptions, we designed and synthesized aryl piperazine-based constrained analogs of NVP-DPP728 in which proline mimetics (pyrrolidine, thiazolidine, (R)-2-methylpyrrolidine etc) at P_1 site may enhance chemical stability [3] and aryl piperazine moiety at P_2 site may enhance potency. The piperazine structure of aryl piperazine at P_2 site provides natural constraint. Some of the synthesized compounds showed good DPP-IV inhibitory activity. The details of the study will be presented.

Figure-1



PP -258

Poster Presentations

Formulation and evaluation of Kollidon® SR based floating matrix tablets of labetalol hydrochloride

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ABSTRACT

Aim and objective:

To prepare sustained release gastroretentive drug delivery system (SR GRDDS) of Labetalol Hydrocloride (LBT).

Rationale:

LBT is used in the treatment of hypertension. It is soluble in lower pH of stomach and has minimum solubility in pH range 6 to 10. It has varying bioavailability ranging from 10 to 80 % owing to its instability in alkaline pH of intestine. Increasing gastric residence time of LBT can help in overcoming the problems mentioned above.

Method:

Various concentrations of Kollidon® SR were used to get desired floating behavior and to sustain the release of drug over 24 hours. PEG 6000 was used as channeling agent (CA) in various concentrations. Lactose was used as diluent. Kollidon VA 64 was used in different concentrations to increase the hardness of tablets. Tablets were prepared by direct compression method. Post compression curing of tablets was done by keeping tablets in oven for 1 hour at 60^{0}C. Tablets prepared were evaluated for physical appearance, hardness, friability, floating behavior and in vitro drug release before and after curing of tablets.

Result:

45% Kollidon® SR, 6% PEG 6000 with lactose as diluent gave sustained release over a period of 24hrs and with lag time of 1 min and total floating time of > 24 hrs.

PEG 6000 as CA improved the dissolution rate (DR) which was further enhanced with increase in lactose concentration.

Post compression curing of tablets is important as it stabilized the release of drug, increase the hardness and decrease the floating lag time of tablets.

PP -259

Poster Presentations

Environ-economic, facile, one pot synthesis of 3-nitro-1,2-dihydroxyanthraquinone and 1-hydroxy-9,10-dioxo-9,10-dihydroanthracen-2yl benzoate using microwave irradiation

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ABSTRACT

An efficient method for the exclusive one pot synthesis of 3-Nitro-1,2-dihydroxyanthraquinone and 1-hydroxy-9,10-dioxo-9,10-dihydroanthracen-2yl-Benzoate (An anthraquionone derivative) under microwave irradiation condition. The structure of newly synthesized compounds have been established by analytical data includes elemental analysis, mass spectra, IR spectra and melting point.

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PP -260

Poster Presentations

Synthesis and antihyperglycemic activity of new 2, 4-thiazolidinediones bearing aryl sulfonylurea moieties

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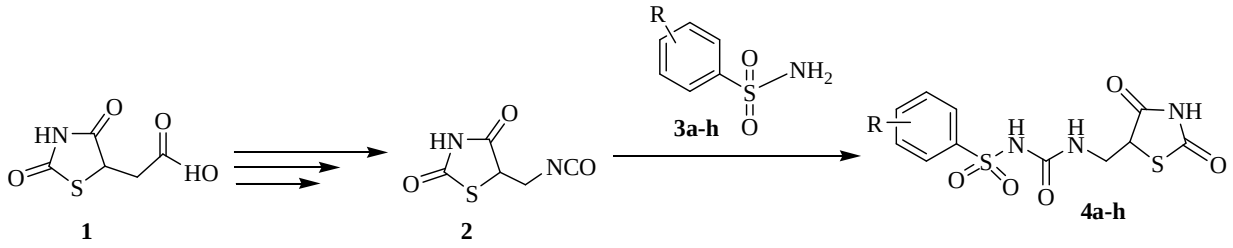
ABSTRACT

New 2, 4-thiazolidinediones with aryl sulfonylurea moieties 4a-h have been synthesized by condensing various substituted sulfonamides 3a-h and á-isocyanomethyl-2, 4-thiazoldinedione. The á-isocyanomethyl thiazolidinedione 2 was obtained by using Curtius rearrangement, starting from known 5-carboxy-2, 4-thiazolidinedione 1. The newly synthesized compounds 4a-h have been evaluated for the antihyperglycemic activity in normal as well as streptozotocin-induced diabetic rat models and among these compounds 4b, 4c, 4e and 4f have shown significant antihyperglycemic activity in sucrose loaded rat model.



Scheme 1. Synthesis of 1-((2, 4-dioxothiazolidin-5-yl) methyl)-3-benzenesulfonyl urea

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PP -261

Poster Presentations

Baker's Yeast: An unique biocatalyst for the synthesis of biodynamic heterocycles

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ABSTRACT

Baker's yeast is a unicellular fungus (*Saccharomyces cerevisiae*) and has been well explored in synthetic organic chemistry.[1] It is readily available, inexpensive and selective biocatalyst. Due to these important aspects synthetic chemists have been taking keen interest in using bakers yeast as a "green biocatalytical reagent" for variety of organic transformations. Baker's yeast catalyzed stereoselective reductions of numerous ketones is the valuable methodology and very popular among synthetic and medicinal chemists. Bakers yeast also found to catalyze other reactions like reduction of double bonds, acyloin condensation, oxidation of thiols to disulfides, hydrolysis of esters etc.[2]

Though bakers yeast has been extensively used in organic syntheses then also there is least attention on its use as a catalyst in accelerating cyclocondensations leading to value added heterocycles.[3]

Considering the dire need of biocatalysis in organic synthesis and to explore the catalytical behavior of bakers yeast in cyclocondensations, here we have carried some cyclocondensations [4,5, 6] for obtaining important bioactive heterocycles, *Viz.* benzothiazoles, 4-thiazolidinone, 4H-Pyran and benzothiazine. The details of the work will be presented.

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PP -262

Poster Presentations

New access to fluorine-containing cyclic α-amino acids *via* electrophilic additions to cyclic *N*-acyl enamines

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ABSTRACT

Fluorination of amino acids brings unique properties, such as high lipophilicity, non-linearly increasing steric demand and (stereo)electronic effects due to the high electronegativity of fluorine atom.(1) Yet incorporation of fluorinated residues into peptides has shown some advantages: decrease in the proteolytic degradation rates, and hence improved *in vivo* absorption and drug permeability through cell membrane. It may also lead to some unexpected conformational biases. These effects depend on nature and position of the fluorinated substituent.(2)

Pipecolic acid, a non- proteinogenic six membered ring homologue of L-proline, is increasingly involved in drug development, either as a scaffold or as a substitute for proline.(3), (4) Here we report on the synthesis of both 3 and 5-Fluoropipecolates; the methodology employed relies on the sequence, electrophilic fluoromethoxylation (or fluorohydroxylation), and subsequent reductive demethoxylation (dehydroxylation) of simple piperidine- or pipecolate-based enecarbamates. The same pipecolate-based enecarbamate can be easily converted to the 5,5-difluoropipecolate, through the corresponding ketone. 5-Mono and 5,5-difluoropipecolates were then coupled with N-Boc glycine, thus leading to model dipeptides whose conformational equilibrium, between the two amide rotamers, was investigated by NMR analysis.

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PP -263

Poster Presentations

Biocatalytic synthesis sugar-PEG based polymeric architectures for drug delivery applications

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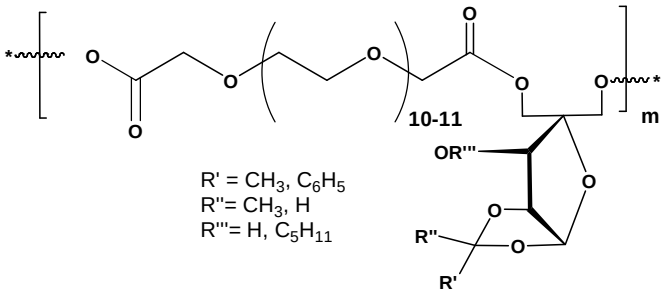
ABSTRACT

Delivery of water insoluble drugs and improving their pharmacokinetic profile are among the major challenges in drug delivery. PEGylation have been proved to be a successful approach to drug delivery due to excellent water solubility and high biocompatibility of PEG unit. The effectiveness of a drug carrier is determined as its ability to control the time over which drug release occurs or to trigger the drug release at specific location or time. Change in pH has been exploited as a useful stimulus in the development of a drug carrier. In the recent past, several pH responsive block copolymeric systems have been designed and studied for their self assembling properties and holding & release of hydrophobic drugs. So far, sugar-PEG polymeric systems have not been explored much for pH responsive drug delivery applications.

Here, we discuss the biocatalytic synthesis of novel sugar-PEG based copolymeric systems bearing acid cleavable group. It included first, the synthesis of 4-hydroxymethylated-1,2-O-arylidene/ isopropylidene-xylofuranose derivatives. These 4-hydroxymethylated sugar derivatives were successfully polymerized with PEG dimethylester using Novozyme-435. All the biocatalytically synthesized sugar-PEG based copolymers have been studied for their molecular aggregation behaviour in aqueous medium. The polymeric aggregates were further explored for their drug encapsulation properties in aqueous solution using nile red as hydrophobic model compound. Nile red release study was performed at acidic pH 5 by means of fluorescence spectroscopy. Details of the studies will be presented in the meeting.



PP -264

Poster Presentations

Synthesis and biological studies of 5-cyano-4(3h) pyrinidinone derivatives

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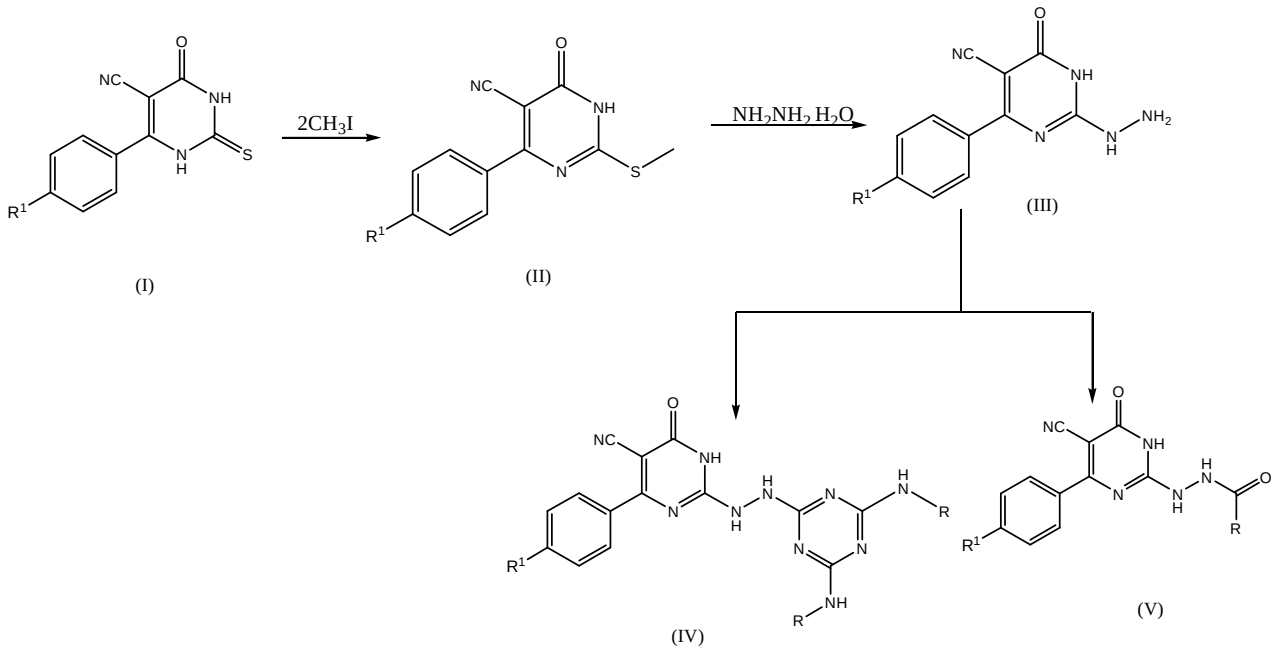
ABSTRACT

Pharmacological study of some 5-cyano-4(3H) pyrimidinone derivatives their arylamides and alkyl/ arylamino s-triaziyl hydrazing derivatives was carried out by preparing and screening them for their antitubercular, antibacterial and antifungal activities. The biologically active function derivatives of the title compound were synthesised from 5-cyano-2-thiouracil. The chemical structure of the compounds was elucidated with the help of elemental analysis, IR and PMR spectroscopy. The antimicrobial activity observed was carried out by cup-plate method at a concentration of 40µg. The significant antitubercular activities of these derivatives were screened by TAACF the Southern research institute. The primary assay summary report showed significant antitubercular activity for some of the compounds but failed in the cytotoxicity test in VERO cells.



Where R^1 = X and R = Alkyl/Aryl -ring.

PP -265

Poster Presentations

Synthesis, spectroscopic characterization and bio-chemical studies of novel organotin(IV) complexes with 2-acetylpyridine-*N*(4)-cyclohexyl thiosemicarbazone

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ABSTRACT

Six new organotin(IV) complexes with 2-acetylpyridine-*N*(4)-cyclohexyl thiosemicarbazone [HAPCT, (1)] ligand of the type [$MeSnCl_2$(APCT)] (2); [$BuSnCl_2$(APCT) (3); [$PhSnCl_2$(APCT)] (4); [Ph_2SnCl(APCT)] (5)]; [Ph_3Sn(APCT)] (6) were synthesized by direct reaction of organotin(IV) chloride(s) with the ligand (1) in an absolute methanol in 1:1 mole ratio under nitrogen atmosphere. The ligand (1) and its organotin(IV) complexes (2-6) have been characterized by CHN analyses, molar conductivity, UV-Vis, FT-IR and ^{1}H and ^{13}C-{^{1}H} NMR spectral studies. The molecular structure of (2) has also been determined by the single crystal X-ray diffraction method. The single crystal X-ray diffraction studies of the complex [$MeSnCl_2$(APCT)] (2) revealed that the ligand (1) acted as uninegative tridentate nature and is coordinated through pyridine-N, azomethine-N and thiolato-S atoms to tin(IV) atom, which is exhibited strongly distorted octahedral coordination. The cytotoxicity of the free substituted thiosemicarbazone ligand (1) as well as its organotin(IV) complexes (2-6) has been evaluated using *Artemia Salina* (Brine Shrimp). The results showed that the organotin(IV) complexes (2-6) were found to be more cytotoxic than the free substituted thiosemicarbazone ligand (1).

PP -266

Poster Presentations

Synthesis and characterization of n-butyl 4- (3, 4 - dimethoxyphenyl) – 6 – methyl – 2 – thioxo – 1,2,3,4 tetrahydropyrimidine – 5 – carboxylate nanoparticles using w/o microemulsion technique

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ABSTRACT

Various pyrimidine derivatives are well known for their properties like antiviral, antitumor, anti-bacterial, anti-inflammatory, anti-hypertensive, anti-cardiovascular agents etc. The n- Butyl 4-(3, 4 - dimethoxyphenyl) – 6 – methyl – 2 – thioxo – 1,2,3,4 tetrahydropyrimidine – 5 –carboxylate was synthesized by using n – butylacetoacetate. The n – butyl acetoacetate was obtained by transesterification of ethyl acetoacetate with n – butyl alcohol and â – keto ester was obtained by Biginelli condensation. The nano particles of n- Butyl 4-(3, 4 - dimethoxyphenyl) – 6 – methyl – 2 – thioxo – 1,2,3,4 tetrahydropyrimidine – 5 –carboxylate were synthesized by water/oil micro – emulsion technique. The average particle size was calculated from the powder X-ray diffraction (XRD) pattern by applying Scherrer's formula. The nanoparticles of n- Butyl 4-(3, 4 - dimethoxyphenyl) – 6 – methyl – 2 – thioxo – 1,2,3,4 tetrahydropyrimidine – 5 –carboxylate were observed by transmission electron microscope (TEM). The diameter of the nanoparticles varied from 15 nm – 65 nm. The nanoparticles were also characterized by FT – IR spectroscopy, TG – DTA – DSC and mass spectroscopy. The n – butyl THPM nano-particles were stable up to 130 °C. The results are discussed.

PP -267

Poster Presentations

Synthesis and characterization of 5-isopropyl-2-phenyl-2,4-dihydro-3H-pyrazole-3-one nano particles by using w/o microemulsion technique

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ABSTRACT

The synthesis of pyrazoles is of great interest due to their wide applications in the pharmaceutical and agrochemical industry. Pyrazole derivatives were reported to possess significant antibacterial, MAP kinase inhibitory, monoamine oxidase inhibitory, insecticidal, anticancer and anti-HIV activities. Pyrazole derivatives are found to possess potent activities such as anti-inflammatory, antimicrobial, antiallergic, antidiabetic, cardiovascular and diuretic. The 5-isopropyl-2-phenyl-2,4-dihydro-3H-pyrazole-3-one was synthesized by using mixture of methyl-isobutylacetate and phenylhydrazine in methanol with the presence of a few drops of acetic acid. Light yellowish crystalline powder was obtained, which was further used to synthesize nano particles by water/oil microemulsion technique. The 5-isopropyl-2-phenyl-2,4-dihydro-3H-pyrazole-3-one solution in chloroform was used in the synthesis of nano-particles. The phase diagram was constructed and the single phase region was identified for the suitable condition to synthesize nano particles. The synthesized nanoparticles of 5-isopropyl-2-phenyl-2,4-dihydro-3H-pyrazole-3-one were observed by transmission electron microscope (TEM). The diameter of the nanoparticles varied from 11 nm – 42 nm. The nanoparticles were also characterized by FT – IR spectroscopy and mass spectroscopy. From the FTIR spectroscopy study C-H, C=C, =N-N- and –C=O bonds were confirmed. The mass spectroscopy indicated the proper fragmentation and mass of the substance. The results are discussed.

PP -268

Poster Presentations

N-Methyl pyridinium tosylate ionic liquid (NMPyTs) mediated convenient synthesis for dihydropyrimidinones

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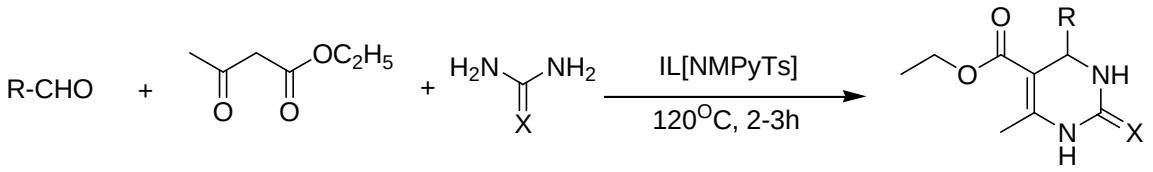
ABSTRACT

3, 4 - Dihydropyrimidinones and thiopyrimidinones are well explode as therapeutic agents. The Biginelli reaction has been widely used for obtaining various derivatives of pyrimidinones. Several efforts are found to be directed to expedite and to provide non tedious reaction conditions for Biginelli reaction. All the efforts are found to require longer unpracticable heating and needs corrosive solvent. In view of the above lacunae here a convenient synthetic protocol has been developed to carry cyclo condensation of multicomponents mediated by freshly prepared N-methyl pyridinium tosylate, safer recyclable ionic liquid. The details of the protocol will be presented.



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PP -269

Poster Presentations

Synthesis of a family of fluorescent molecular sensors and study on their anion recognition property with a large number of anions

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ABSTRACT

Design and synthesis of molecular receptors capable of detecting the presence of specific ion has received considerable interest in recent years. Among various receptors, fluorescent molecular sensors, which can be constructed by the combination of a recognition moiety with an optical or electronic transduction unit is of special interest because of their high sensitivity and quick response. To design fluoroionophores, photoactive organic and inorganic compounds can be used as fluorophore and organic moiety, which can interact with incoming ions can be used as ionophore. For the recognition of anions, various noncovalent interactions, such as hydrogen-bonding, electrostatic, hydrophobicity are mainly considered. With a view to develop molecular sensors for anions, we have prepared a series of fluoroionophores comprising Ru(II)-polypyridyl based fluorophore and modified 2,2'-bipyridine/1,10-phnanthroline as ionophore. All these complexes have been characterized on the basis of analytical and spectroscopic methods. Anion recognition property of these complexes have been investigated with a large number of anions (H2PO4-,Cl-, Br-, NO3-,F-, OAc-,ClO4-,BF4-,I-) and the recognition event was monitored by flurescence, UV-Vis and 1H NMR spectral change. Among these anions, F-, OAc- and H2PO4- exhibit strong interaction, the binding constants were calculated on the basis of fluorescence titration data. All of these results and the energy/electron transfer process involved in the recognition event will be presented.

PP -270

Poster Presentations

Cation-induced fluorescent excimer formation in calix[4]arene-chemosensors bearing quinoline moiety: experimental, molecular modeling and crystallographic studies

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ABSTRACT

The development of molecular sensors for efficient detection of specific metal ion is an emerging area in chemistry because of their potential analytical applications in many different fields, including chemistry and biology. In this regard, detection by fluorescent technique has been widely used because of some distinct advantages in terms of sensitivity, selectivity, response time, in-situ monitoring etc. This method of detection requires fluoroionophores, which are composed of ion recognition unit, known as ionophore, and a fluoregenic unit as probe, the photophysical property of which perturbs during the recognition process producing changes in luminescent emission. Another approach of designing fluoroionophores is the addition of two fluorophores containing flexible aromatic moieties so that interaction with metal ion brings the fluorophores close enough (within Vander Waals contact) to make weak interaction such as π-π stacking. Under this condition, electronic excitation of one ring can cause an enhanced interaction with its neighbor, leading to what is termed as excited-state dimer or excimer. This excimer typically provides a broad fluorescence band with the maxima at lower energy compared to emission from monomer and this band can be used to read out the molecular recognition process more conveniently.

A number of calix[4]arene based chemosensors containing quinoline moiety as fluorophore have been synthesized. These fluoroionophores have been designed with variation in substituents at the upper and lower rims and the calix moiety in these compounds exist in cone and 1,3-alternate conformation, as confirmed by single-crystal X-ray study. Ion-binding property of these molecules has been investigated with a large number of cations and anions. Strong quenching of monomer emission and formation of excimer is observed in presence of Hg^{2+}, Pb^{2+}, Fe^{3+} and Cu^{2+}, however no excimer emission is noted for F^-. Binding constants have been determined using fluorescence titration data. Molecular modeling studies performed by molecular mechanics force field (MMFF94) using Monte Carlo search method and DFT calculations predicted the observed excimer formation for selective metal ions.

PP -271

Poster Presentations

Synthesis and characterization of novel methylene derivatives of sydnones as antimicrobial agents

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ABSTRACT

Ten different Mannich bases were synthesized and characterized by IR, NMR spectroscopy and elemental analysis. The synthesized compounds were evaluated for their antibacterial and antifungal activity. Some of the compounds were found to possess excellent activity against tested organisms.

PP -272

Marine ayurvedic medicinal plants : emerging target for NCE?

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ABSTRACT

It's a known fact that marine biodiversity consists of 2/3 of total biodiversity of the Earth. The territorial biodiversity is being explored for many of the successful new chemical entities e.g. Reserpine, Taxol, Guggalu sterol etc. to name a few majority of the medical plant has been explode for such objectives. Traditional medical systems are viewed as the potential source for such a development; ayurveda is the oldest 'Ancient medical system' being popularized due to many of its unique aspects throughout the World. Most of these aspects are being explored scientifically worldwide to fulfill contemporary health requirements. However little attempt was made to explore marine Ayurvedic medicinal plant for possible NCE.

This poster deals with detailed phytochemical review of the known marine Ayurvedic medicinal plants. It may develop new area of focus for phytochemical research in this emerging field

PP -273

Poster Presentations

Trends in research on plant alternative oxidase

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ABSTRACT

A portion of respiration in plant mitochondria, active under conditions of biotic and abiotic stresses, is known to be insensitive to cyanide. The product of reduction of oxygen consumed by this alternative respiration is hydrogen peroxide (H_2O_2), a reactive oxygen species (ROS), as opposed to the water molecule [1]. Reactive oxygen species are now recognized as important signal molecules in diverse metabolic processes. An enzyme, ubiquinol oxidase that coexists with cytochrome oxidase and uses reduced ubiquinone, a substrate common to both, is inhibited by salicylhydroxamic acid (SHAM) and has become known as alternative oxidase [2]. Since no protonmotive force is generated during activity of AOX, electron flow through AOX is presumed to dissipate energy without any ATP synthesis. Therefore, activity of AOX is regarded as "waste of energy" [3]. Plant mitochondria have never been regarded as a major site of H_2O_2 production, with the premise that AOX reduces oxygen to water. ROS have been suggested as signaling molecules in the crosstalk between organelles and the nucleus. However, much remains to be established, especially initiation of mtROS generation [4,5]. Recent development has added to the understanding of the position of AOX in plant physiology [1]. Does AOX activity play a role in redox homeostasis that caters to the temporal and spatial needs of the cell?

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PP -274

Poster Presentations

Design and synthesis of 1-(2-amino-1-(4-methoxyphenyl) ethyl) cyclohexanol analogs as potential microbial agents

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ABSTRACT

Azetidinone 5a-g derivatives were prepared from the reaction of Schiff base and chloroacetyl chloride and in presence of triethylamine. The structures were assigned on the basis of elemental analysis, IR, ^{1}H NMR ^{13}C NMR and Mass spectral data. All the compounds were screened against different strains of bacteria and fungi. Compounds 4a, 4b, 4d, 4e, 4f, 5b, 5e and 5f possessed very good activity against bacterial and fungal species.

PP -275

Antimicrobial studies of triazolo trianzino indoles by agar dilution method

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ABSTRACT

Azoles and azines are well known for their diverse biological activities. It is also known that fusion of the heterocyclic nuclei enhances the pharmacological activities more than the parent nucleus. The importance of the indole nucleus is well established in pharmaceutical chemistry (Holla, 2002), (Babalola, 1998). A few naturally occurring members of this class of compounds, pyridindolol and the two antibiotics CV-1 and guatamicin have been isolated from different species of streptomyces. Triazolo trianzino indoles show antihypertensive, antiviral, blood platelets aggregation inhibitory, analgesic and antibacterial activities (Abdul-Latif, 1989). Several as – triazines fused with an indole nucleus have been considered as potential drugs for the treatment of common cold infections caused by several rhino virus strains. These compounds were active in nitro not only against rhinovirus but also against Coxsockie, Echo, Herpes, polio, Pseudorabbies and vaccinia viruses (Scott and Baginski, 2000). 1-Substitutedphenyl-10H-[1, 2, 4]triazolo[3', 4': 3, 4] [1, 2, 4]triazino[5, 6,-b] indoles,the whole series was investigated for their antimicrobial activity profile using Agar Dilution Method. Minimum inhibitory concentration of each compound was detected against various bacterial strains and fungal strains with standardized method by NCCLs.

PP -276

Poster Presentations

A molecular dynamics study of HIV-integrease towards anti-HIV drug discovery

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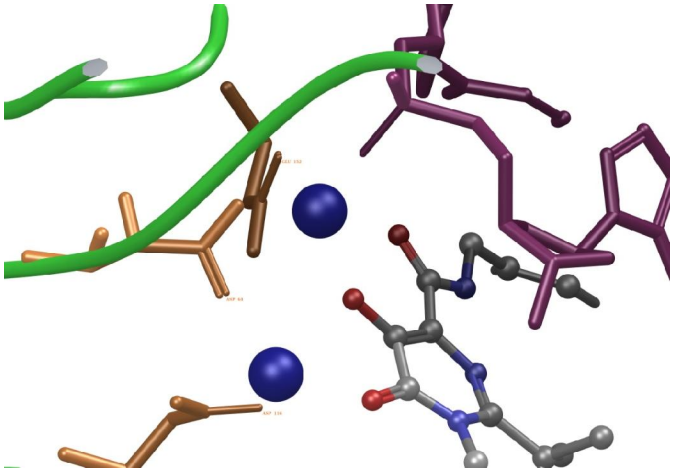
ABSTRACT

The successful anti-HIV drug discovery exists, however resistance and cross resistance possess major threats and needs attentions. The only approved drug raltegravir (FDA 2007) is currently available to target this vital virally encoded enzymes "HIV Integrase". The unavailability of complete X-ray crystal structure makes hurdles to understand the catalytic information of this key enzyme. Therefore the present work is the development and molecular dynamics calibration of 3D catalytic model of HIV integrase towards anti-HIV drug discovery.

There is a lack of complete model giving a detailed account of structural catalysis information by integrase and drug resistance. Therefore, here we describe a creation of integrase model using homology followed by global minimization, validated by experimental facts. The molecular dynamics studies were further extended to understand the molecular recognition phenomenon of INSTIs.

The present studies clearly demonstrate the catalytic mechanism of potential molecules as INSTIs. The structural study and simulation provides insight for new drug discovery through the graphical and empirical co-relation in comparison to biochemical results.



PP -277

Poster Presentations

Synthesis and MIC of 3-(4'-phenylsulphonamidophenyl)-5-aryl-isoxazoles

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ABSTRACT

The isoxazole derivatives possess therapeutic activity like bactericidal, insecticidal, fungicidal, etc. They are also widely used as anesthetic, analgesic and antidiabetic agents. Some new isoxazole derivatives have been prepared by the condensation of 4'-phenylsulphonamidochalcones with hydroxylamine hydrochloride. The structure of the products has been characterized by elemental analyses and spectral studies .The products have been screened for their antimicrobial activity using different strains of bacteria and fungi .Two compounds of the series were found very active against some bacterial and fungal strains .They were further tested for tertiary screening to find exact MIC.

PP -278

A validated chiral LC method for the enantiomeric separation of duloxetine hydrochloride using chiral-AGP as the stationary phase

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ABSTRACT

The present work describes the development and validation of chiral HPLC method for the enantiomeric separation of Duloxetine hydrochloride [*(S)*-N-Methyl-3-(1-naphthalenyloxy)-3-(2-thienyl)propanamine], an antidepressant drug. The enantiomers of Duloxetine hydrochloride were baseline resolved on a Chiral-AGP (150 mm × 4.0 mm, 5 µm) column using a mobile phase consisting of acetate buffer (pH 3.8; 10 mM)-acetonitrile (93:07, v/v) at a flow rate of 1.0 mL/min. Interestingly, distomer was eluted prior to eutomer in the developed method. The optimum conditions of resolution were established by systematically studying the effect of organic modifier, pH of buffer, concentration of buffer and column temperature. The thermodynamic parameters were also calculated. The developed method was extensively validated. Thus, the limit of detection and limit of quantification of *(R)*-enantiomer were found to be 150 and 400 ng/mL, respectively, for 5 µL injection volume, whereas the method precision for *(R)*-enantiomer at limit of quantification level was within 1.4 % R.S.D. The recovery of *(R)*-enantiomer was within 105 % in bulk drug. The proposed method was found to be suitable, precise and accurate for the quantitative determination of *(R)*-enantiomer in bulk drugs.

PP -279

Poster Presentations

Computer-aided design of novel competitive inhibitors bearing drug-like properties for *schistosoma mansoni* hypoxanthine guanine phosphoribosyl transferase

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ABSTRACT

Schistosomiasis is a chronic, debilitating, major human parasitic disease caused by trematode parasites of the genus *Schistosoma* infecting over 200 million people in more than 74 countries throughout the world (Bergquist, 1995; Bergquist and Colley, 1998). The existing anti-schistosomal drugs have dire side effects (Ribeiro-dos-Santos et al, 2006). There are also reports of *Schistosoma mansoni* becoming resistant to drugs, owing to which development of an alternate drug with sufficient efficacy and safety is necessitated. In effect to which homology modeling of Hypoxanthine Guanine Phosphoribosyl Transferase (HGPRT) of nucleotide salvage pathway of *S. mansoni*, a good anti-schistosomal drug target (Dovey et al, 1986; Kanaaneh et al, 1994; Kanaani, et al, 1995), was carried out with HGPRT of *Toxoplasma gondii* as template using SWISS-MODEL (Schwede et al, 2003). Inhibitors for *S. mansoni* HGPRT were designed *de novo* using HyperChem and evaluated for their molecular properties and drug likeness using 'Molinspiration' (http://www.molinspiration.com/cgi-bin/properties/), an online tool and for mutagenicity, using 'Ames Mutagenicity Prediction' tool (http://www.chembiogrid.org/cheminfo/rws/ames/), another online tool. Molecular docking simulations of designed inhibitors with *S. mansoni* HGPRT and human HGPRT were carried out using FlexX (Kramer et al, 1999). Inhibitors 'inh2' and 'inh7' showed ADME properties within the acceptable range (Lipinski et al, 2001) and were predicted to be non-mutagenic in nature. Inhibitors 'inh2' and 'inh7' were found to bind *S. mansoni* HGPRT more strongly than the natural substrate of *S. mansoni* HGPRT, viz., Alpha-D-5-Phosphoribosyl-1-Pyrophosphate (PRPP), showing that they are competitive inhibitors of *S. mansoni* HGPRT. Also, 'inh2' and 'inh7' were found to interact with many of the PRPP-binding residues of *S. mansoni* HGPRT. Further, binding of 'inh2' and 'inh7' to human HGPRT with a significantly less favourable binding energy than PRPP, besides not binding to any of the PRPP-binding residues, showed that they are not competitive inhibitors of human HGPRT. Therefore, 'inh2' & 'inh7' were found to be good drug candidates for *Schistosoma mansoni* infection.

PP -280

Poster Presentations

Synthesis and characterization of some novel benzothiazole derivatives

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ABSTRACT

The Benzothiazole ring system is having phenyl ring fused with thiazolering.The study of benzothiazole derivatives are of considerable interest due to their important biological properties. A series of potent and selective antitumor agents mostly from substituted 2-(4-aminophenyl) benzothiazoles were developed and examined, in vitro, their antitumor activity in ovarian, breast, lung, renal and colon carcinoma human cell lines[1] and found that the activity of different derivatives are good. So derivatives of benzothiazoles were synthesized, named5-arylidene-3-(6-fluorobenzo[d]thiazol-2-yl)-2-iminothiazolidin-4-one, from most common organic liquid compound 4-fluoroaniline,in four steps and further characterized by MASS, IR, ^{1}H NMR and ^{13}C NMR spectral data.

PP -281

Microbiological approach for the reduction of organic pollutants from soil

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ABSTRACT

Microbiology deals with the detailed understanding and studies of microbial activities which are helpful in mitigation or reduction of various pollutants.Microbial communities perform enormous tasks mainly to keep themselves perpetuating in their ecosystems.Their activities like photosynthesis,respiration and breakdown of organic matters into simpler inorganic moieties are carried out for survival.These bioactivities play a pivotal role in attaining a dynamic equilibrium of the earth's ecosystem.Pollutants like petroleum and organic chemical, due to their hydrophobic nature, are not easily degraded for a long time period. As they are mutagenic and carcinogenic it is utmost important either to remove or to transform them into innocuous form.

Efforts have been made for the screening and development of microorganisms that can degrade organic pollutants from the soil. Various soil samples have been collected from the petroleum contaminated sites and studied with reference to physicochemical and microbiological parameters. Selected strains were further checked for their ability to degrade poly aromatic hydrocarbons like napthalene and phenanthrene. Strains were developed through adaptation and mutagenesis. Selected isolates have been examined for their growth and biodegradative ability on various cheaper substrates to make them potential and promosing candidate for bioremediation of such organic pollutants.

PP -282

Poster Presentations

Novel substituted quinolinyl benzimidazoles as potential hypoglycemic compounds

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ABSTRACT

Diabetes (Type-II) is a disease characterized by insulin resistance hyperglycemia and hyper insulinemia , leading to impaired secretion of insulin in latter stages. Diabetes if often associated with obesity, dyslipidemia and hypertension which are collectively known as syndrome X or insulin resistance associated disorders (IRDA). Current therapies for type-2 diabetes have inherent problems of non compliance, resistance and hypoglycemic cascade with insulin and sulphonyl ureas .Different types of PPAR agonists have been shown to have beneficial effects on described characteristics of type-2 diabetes .Glitazones type therapies are in market but some of them reported to be hepatotoxic. Therefore more effective and better tolerated novel antidiabetic agents are needed.

The antidiabetic activity of various heterocyclic systems[1] has been reported by several schools of research. Some imidazoline derivatives have shown promise as potent hypoglycemic agents. Ischilawa e. al.[2] reported that some derivatives of substituted 2 – imidazoline possessed stronger hypoglycemic activity than that of tolbutamide. These researchers[3] have synthesized derivatives of 2-(benzhydrylimino)-imidazoline and 1,3-substituted imidazolines and reported them to be useful as oral hypoglycemic. The hydrochloride and hydroiodide salts of these imidazolidines have shown higher hypoglycemic activity than that of hypoglycemic activity of tolbutamide and phenformin in experimental animals. Schweitzer[4] reported 2 – imino – 1 – phenyl – sulphonyl – imidazolidines as hypoglycemic in rats at a dose level of 10 mg/kg orally. The exact mechanism of action of benzimidazole derivatives as antidiabetic agents is not known, however it is thought that these compounds promote penetration of glucose and other sugar materials in to muscles and fats.

Therefore it was thought worthwhile to synthesise some new substuted benzimidazole derivatives by incorporating substituted cyclic amino moieties at 7-position of benzimidazoles with a hope to get better novel antihypertensive agents.

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PP -283

Poster Presentations

In-vitro and *in-vivo* evaluation of antidermatophytic activities of some medicinal plants used by the rural and tribal people of N. E. Region of india

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ABSTRACT

Fungal infections particularly involving the skin and mucosal surfaces constitute a serious problem in tropical and subtropical developing countries (Stern 1996). Skin diseases, especially dermatophytoses, are an important problem in India (Prasad *et al.* 2004). Dermatophytoses are common superficial cutaneous fungal infections caused by filamentous fungi such as *Trichophyton, Microsporum* or *Epidermophyton* species which have the capacity to invade keratinous tissues, such as hair, skin or nails, of humans and animals (Weitzman *et al.* 1995). Although a large number of synthetic allopathic drugs are available to treat dermatophytosis, the increasing incidences of fungal resistance towards these synthetic drugs combined with their associated side effects like gastrointestinal disturbances, cutaneous reaction, hepatotoxicity, leucopenia etc. forced scientists to search for new antimicrobial substances from natural sources (Del Aguila *et al.* 1992, Torok *et al.* 1993, Lopez-Gomez *et al.* 1994, Gupta *et al.* 1998). People now are opting more for natural origin drugs. Based on the ethnobotanical knowledge and local use of some plants, an attempt has been made to assess the antidermatophytic properties of four plants- *Trachyspermum ammi, Cinnamomum porrectum, Piper betle Linn., Allamanda cathertica Linn.* and their (w/w) combination against five species of dermatophytes *viz. Trichophyton mentagrophytes*, *Trichophyton rubrum*, *Trichophyton tonsurans*, *Microsporum gypseum* and *Microsporum fulvum*. The inhibition zones were determined by Agar cup diffusion technique (Adamu et al. 2006). *In-vitro and in-vivo* results (Individual as well as the mixed formulation) are very encouraging. MIC values (ranging between 0.312-0.625 μg/ml) are close to standard drug as determined by two fold serial dilution method.

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Poster Presentations

Harnessing C3-symmetric molecules in service of mankind: application as carrier of drugs

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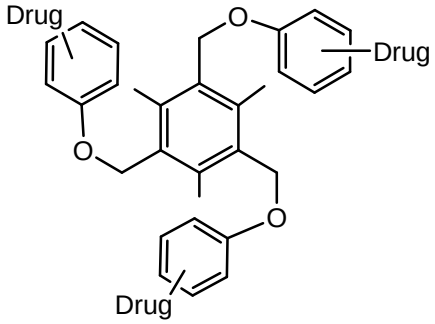
ABSTRACT

One of the most important applications of synthetic organic compounds is their utility in treatment of various diseases. They are useful in treating metabolic disorders as well as in curing some lethal and chronic ailments such as tuberculosis, leprosy, cancer, diabetes, hypertension etc. Tuberculosis is one of the wide spread disease in countries like India. There are several therapeutic agents in use for its treatment which requires longer period stretching from few months to a couple of years.

C3-symmetric molecules are special for various reasons [1] and they have been synthesised for some important applications such as asymmetric catalysis and chiral recognition [1,2]. They have also been applied as metal binding ligands [3] and are also useful in preparation of dedritic molecules [4]. In continuation with our interest in synthesis and applications of C3-symmetric small molecules [5], herein we report our ongoing work on utilisation of C3-symmetric compounds as drug delivery systems.

The C3 symmetric templates have been designed to be employed as carriers of some important drugs and are expected to affect a controlled three fold release of the attached drugs in the body. To begin with, we have synthesised some new C3- symmetric compounds as carriers of anti-tubercular drugs such as INH. Their anti-tubercular activity and pharmacokinetics studies are being persuaded.



PP -285

Poster Presentations

Synthesis and antimicrobial activity of 3-aryl-5-(4' N,N- dimethyl amino phenyl)-1-H/ $COCH_3$ pyrazolines

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ABSTRACT

4 N,N-Dimethyl amino phenyl Benzaldehyde1 on treatment with different acetophenones yielded 1 Aryl-3-(4"N,N-dimethylamino Phenyl)-2- Propenone (2a-j) which on cyclisation with hydrazine hydrate gives 3 Aryl-5-(4' N,N-dimethyl aminophenyl)-1-H/acetyle pyrazolines (3a-j,4a-j). The structures of the compounds 2a-j,3a-j,4a-j were confirmed by elemental analysis, IR,NMR &MASS spetral data. All the products were evaluated for their in vitro growth inhibitory activity against several microbes.

PP -286

Photocatalytic degradation of pyrogallol by fenton's, photo-fenton's re-agents in presence of titania: a waste water treatment process

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ABSTRACT

The commonly used waste water treatment processes include adsorption, oxidation, photo catalysis, biological methods etc. The oxidation process involves the use of oxidants, which may remain in soluble form adding another facet of water pollution. However, Photo- catalytic treatment of polluted water holds good promise as it utilizes insoluble semi conducting powder, which mineralizes the organic pollutants. A search is still on for an alternate method of treating waste water with such active species so that the water is not further polluted after the removal or degradation of pollutants. Here Fenton's reagent enters the scene. In recent years, various photochemical methods for the destruction of organic pollutants in waste water have been developed. The photo-catalytic degradation of pyrogallol over titanium dioxide using photo-Fenton and other related reagents was investigated. The effect of various parameters such as pH, concentration of pyrogallol, amount of semiconductor, amount of H_2O_2,concentration of ferric ions, light intensity etc. were observed. The photo-catalytic degradation of pyrogallol follows pseudo first order kinetics. A tentative mechanism Department of chemistry has been proposed for the photo-catalytic degradation of pyrogallol using photo-Fenton's reagent.

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Poster Presentations

Synthesis of some novel 4-thiazolidinones as potential antitubercular agents

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ABSTRACT

The starting compound 5-nitro benzimidazol -2'-yl-o-benzoyl hydrazide, on treatment with aromatic aldehydes yielded the corresponding benzal-(5'-Nitro benzimidazol-2'-yl-o-benzoyl) hydrazines 2a-o. The heterocyclisation of 2a-o with thioglycolic acid and thiolatic acid furnished the corresponding 2-aryl-3-(5'-nitro benzimidazol -2'-yl-o-benzamido)-5-H-4-thiazolidinones 3a-o and 2-aryl-3-(5'-nitro benzimidazol-2'-yl-o-benzamido)-5-methyl -4-thiazolidinones 4a-o.

The compounds were screened for their antitubercular activity against mycobacterium tuberculosis H37RV.

PP -288

Synthesis of bis and mixed heterocycles using green methodologies and their biological activities

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ABSTRACT

Heterocyclic compounds display a wide variety of biological properties, many of which can be exploited for medicinal purposes and are also essential for the human well-being. Therefore methods for the synthesis of such systems are of significant interest. The environmental protection has become a global concern and the synthetic organic chemists are searching the ways of developing and applying more efficiently and environmentally benign strategies for future sustainable growth. One of the thrust areas for achieving this target is use of Green methodologies in Organic Synthesis. In recent years, Microwave Assisted Organic Synthesis (MAOS), Ultrasound Assisted Organic Synthesis (UAOS), Ring Closing Metathesis (RCM), Aqueous Phase Organic Synthesis (APOS), Solvent Free Organic Synthesis (SFOS), Enzyme Catalyzed Organic Synthesis (ECOS) attracted the attention of organic chemists. The salient features of these methodologies are enhanced reaction rate, easy workup, high yields, operational simplicity, greater selectivity and experimental ease of manipulation, low cost and economy. In view of these advantages of the above environmental benign approaches and as a part of our ongoing research program towards the non traditional methods, the concept of Green synthesis has been adapted for the rapid and efficient synthesis of some bis and mixed heterocycles of biological interest.

PP -289

Poster Presentations

Synthesis of azetidinones as biologically potent agents

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ABSTRACT

Literature survey reveals that 2-azetidinone derivatives possess wide therapeutic activities like sedatives, hypnotic, anticonvulsant and antibacterial activity. In order to explore the therapeutic activities associated with azetidinone, we have synthesized some novel 2-azetidinones and reported their biological screening. Initially condensation of p-acetamidophenoxy acetyl hydrazide with aromatic aldehydes have been undertaken to prepare N^1-substituted benzal, N^2-p-acetamidophenoxyacyl hydrazines. These Schiff's bases are then treated with chloroacetyl chloride to obtain 4-aryl-1-p-acetamidophenoxy acetamido-3-choloro-2-azetidinones.The compounds have been characterized by elemental analysis, IR and NMR spectral study. Among the compounds screened for antimicrobial activity many compound showed significant activity.

PP -290

Acoustical studies of some pyrazole schiff bases in DMF at 308.15K

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ABSTRACT

Density, ultrasonic velocity and viscosity of some pyrazole Schiff bases derivatives have been studied in dimethyl formamide (DMF) at 308.15 K. From the experimental data, various acoustical parameters such as specific Impedance (Z), isentropic compressibility ($\hat{e}_s$), Rao's molar sound function (R_m), Van der Waals constant (b), relaxation strength (r), intermolecular free length (L_f), internal pressure (ð), solvation number (S_n), etc. have been evaluated, which helps in understanding the molecular interactions occurring in these solutions

PP -291

Poster Presentations

Environment- benign procedures for oxidation of Hantzsch 1,4-Dihydropyridines and alcohols/benzylalcohols using green catalysts and green solvent

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ABSTRACT

Room-temperature ionic liquids are gaining academic and industrial world wide attention as these can be used to replace the organic solvents in catalysis, synthesis and separations. The unique properties of RTILs enable their use as alternative solvents and may speed the introduction of potentially "green" solvents into sustainable industrial processes.

Even the development of heterogeneous catalysts for fine chemical synthesis has become a major area of research recently (simplified recovery and reusability and the potential for incorporation in continuous reactors and micro reactors) over homogenous system can make a major impact on the environmental performance of a system. The majority of these novel catalysts are based on silicas primarillay silicas display many advantageous properties such as excellent stability (chemical and thermal), high surface area, good accessibility and catalytic material can be robustly anchored onto its surface to provide catalytic centers. These also consider towards the area of "*Green Chemistry*".

Even in the past several years, there has been dramatic increase in the synthesis of novel "green" ionic liquids (ILs). Chemical engineers have been developing ILs to replace the conventional volatile organic solvents that contribute to the serious air pollution Ionic liquids are class of the chemicals that have potential as benign industrial alternatives; these organic salts have vanishing low vapour pressure and are liquid at ambient conditions and do not evaporate or cause air pollution[2]. Substitution of ionic liquids for traditional organic solvents could potentially improve environmental health and industries could save billions of dollars in future environmental mitigation and clean-up .

en the use of water as solvent (universal solvent) also lead towards the area of *Green Chemistry.*

Oxidation of Hantzsch 1,4-dihydropyridines[5] and the selective oxidation of alcohols/benzylalcohols to the corresponding aldehydes or ketones are the most important reactions in oganic synthesis. These substituted pyridines exhibit a broad spectrum of biological activities such as antibacterial, antischemic activities etc. Moreover, oxidation of alcohols/benzyl alcohols is a fundamental transformation in both laboratory synthesis and industrial production since these products are important precursors and intermediates for many drugs, vitamins and fragrances. Various classical reagents are available for both oxidations but those suffer from certain disadvantages such as toxic nature of reagent, harsh reaction conditions, expensiveness of reagent.

In order to cumbersome those disadvantages, we tried to synthesize greener heterogeneous catalyst and ionic liquid and applied to carry the reactions that fall in the area of *Green Chemistry.*

PP -292

Poster Presentations

Chemical screening of Guggal (*Commiphora wightii*) accessions collected from different natural habitats of Rajasthan

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ABSTRACT

Guggal (*Commiphora wightii* Arnott. Bhandari) is an important medicinal plant which has been used in Ayurvedic medicine - a traditional medicine system practised in India for about 3000 years. The species is naturally distributed in the drier tracts of Rajasthan, Gujarat and M.P. In the present study, twenty three accessions collected from different natural habitats of Rajasthan were used for chemical screening based on guggulsterone-Z. Guggulsterone-Z is one of the important secondary metabolized bio-active molecules which act as an antagonist of the farnesoid X receptor, that result in decreased cholesterol synthesis in the liver. It also inhibits the growth of human prostate cancer cells by causing apoptosis.

Chemical screening and determination of guggulsterone-Z were conducted by High Performance Thin Layer Chromatography (HPTLC) and High Performance Liquid Chromatography (HPLC) methods, respectively. Chromatographic separation was achieved on aluminium pre-coated silica gel 60 F254 plates with chloroform-methanol-formic acid 9.5:0.3:0.2 (v/v/v) as mobile phase for HPTLC study and HPLC separation was achieved on a RP-18 column using mobile phase water-methanol system (65: 35, v/v) and detection was set at UV wavelength of 242 nm. The Ethyl acetate extract of dried stem bark was evaporated and dissolved in methanol. The solution was filtered through a 0.45 μm filter prior to HPLC analysis. Guggulsterone-Z content (mg/g) varied greatly among the accessions and its range was 0.73 $\pm$ 0.12 to 4.19 $\pm$ 0.66. Guggulsterone-Z content was lowest in the accession DMAPR CW 62 and it was highest in the accession DMAPR CW 52.The present study thus serves as an aid for the selection of an elite guggal genotype based on guggulsterone-Z content from the natural habitats of Rajasthan for commercial utilization.

PP -293

Poster Presentations

Synthesis of 7 – Methoxy -2 – Cl – Quinoxaline

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ABSTRACT

Quinazoline and its derivatives are a class of hetero aromatic compounds that have drawn much attention because of their biological and pharmaceutical activities including a wide range of anti tumour activity. They are also found to show remarkable antimicrobial properties against micro – organisms associated with death in patients carrying immuno compromised diseases. Prompted by these observations and taking into consideration the leading anti tumour activity that is responsible for the morbidity and mortality of a large population worldwide and in continuation of our research work in quinazoline chemistry we here in report the synthesis of 7 – methoxy – 2 –Cl – quinoxaline, a highly efficient and versatile synthetic approach to the central core of anticancer quinazolinone derivative. In the present one pot sequence the aryl nitro group is apparently reduced by cyclo condensation to form quinazolinones.

The starting compound was 4 – methoxy – 2 – nitro benzaldehyde. It was reduced into 2 – amino – 4 – methoxy benzaldehyde by the use of Pd and methanol under inert atmosphere at room temperature under hydrogen blender for 12 hours. 2 – amino – 4 – methoxy benzaldehyde after mixing with urea and dissolving in NMP was heated for two hours in R.B.F. in presence of a catalyst to get 7 – methoxy quinazoline – 2 – ol 7 – methoxy quinazoline – 2 – ol was then dissolved in $PoCl_3$. The mixture was heated on oil bath at 140°c for an hour. After 12 – hours the mixture was partitioned between ethyl acetate and saturated $NaHCo_3$. The crude product was purified from ethyl acetate fraction. The yield was 85 % and the purity was 99 %.

The detail about methodology including proposed mechanism will be present at the time of oral presentation.

PP -294

Poster Presentations

Biodegradation of chrysene by marine fungi – an approach for remediation of contaminated marine environment

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ABSTRACT

Chrysene is a four ringed organic pollutant and found ubiquitously in marine sediments and aquifers due to its low water solubility and persistent nature. Microorganisms play key role in degradation of this priority pollutant. For this study, coastal region of Alang is selected due to its extensive ship breaking activities. Samplings were done between the duration of Feb. '09 to Nov. '09 at an interval of three months. Physico-chemical parameters *viz.* pH, Temperature, DO, BOD, Alkalinity, Chloride content, TDS, Na^+ and K^+ content, Phosphorous, Sulphate, Hardness were examined. Nine different fungal isolates having capability to degrade chrysene were obtained by enrichment culture methods. Degradative abilities of isolates for chrysene degradation were detected by two plate assays (i) Sundman & Näse plate assay and (ii) Bavendum reaction during primary screening. Halos around mycilial mats indicated degradative capabilities. The nine isolates were further examined for chrysene degradation in liquid cultures during secondary screening. Experimental conditions kept were: pH (6.5), chrysene concentration (60 ppm), temperature (30 °C), and inoculum size (10^8 spores/mL). Out of nine isolates, three showed highest chrysene degradation on 7^{th} day namely S1-3 (83.08%) followed by S2-3 and S4-2 (77.88% and 71.96% respectively). Optimization of cultural conditions for maximum chrysene degradation using CCD approach of RSM (Response Surface Methodology) is in progress. The isolate would be further exploited for its role in co-culture experiments, enzyme characterization and microcosm experiments to establish its significance in remediation of hydrocarbon contaminated marine environments for sustainability of marine environments.

PP -295

Poster Presentations

Potential of fungi in biotreatment of raw textile wastewaters

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ABSTRACT

Fungal biomasses have great potential for decolorization, detoxification and bioremediation of treating industrial effluents that are highly colored containing toxic aromatic amines. Dyes specially Azo and Reactive dyes when released in water bodies cause several problems as they are highly recalcitrant and carcinogenic having high COD. Elimination of these by physico-chemical methods makes the content more toxic but with biological process toxicity is reduced. A total of 50 fungal isolates were collected from Victoria Reserve Forest, Bhavnagar The effluent was collected from textile mill located near Jetpur (Gujarat). The efficacy of all the isolates was tested by primary and secondary screening for maximum decolorization of textile dye effluent. *Aspergillus* sp. and *Mucor* sp. designated as AJ1 and AJ18 were the most potential organisms. The effect of various cultural parameters such as pH, temperature, inoculum size, carbon, nitrogen, phosphate and nutrient source were optimized for maximum decolorization. The fungi were checked for production of lignolytic enzymes. Further work was done for getting enhanced Laccase activity by optimizing various parameters. Saw dust - a natural substrate induced maximum laccase activity i.e. 0.0203EU/mL (183 mg/50 mL) where the enzyme activity was increased by 75%. This study indicates that pollution and health problems are ever on an increase, treating textile dye effluent with fungi can help in reducing environmental problems. Green technology using fungi can thus be exploited for sustainability of the environment.

PP -296

Poster Presentations

Achromobacter xylosoxidans in remediation of petroleum hydrocarbon polluted saline sites around bhavnagar coast, gujarat, india – a step towards clean technology on the sea coast and sustainable development

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ABSTRACT

Sustainable development requires the promotion of environmental management and a constant search for new technologies to treat vast quantities of wastes generated by increasing anthropogenic activities and global warming. Generated from incomplete combustion of fossil fuels and other industrial activities, Polycyclic Aromatic Hydrocarbons (PAHs) are ubiquitous in environment. In the present study, we analyzed total PAHs present in the soil and sediment samples and isolated a total of twelve efficient halotolerant multiple PAH degrading bacteria. Among these High Molecular Weight PAHs, chrysene, a recalcitrant PAH that has been less studied with respect to PAH degradation, had been selected for further studies as a representative PAH compound. Isolate CG542 exhibited maximum degradation of chrysene i.e., 40.5% on 14th day. The isolate has been identified as *Achromobacter xylosoxidans* based on various molecular and biochemical analyses. On optimization of various cultural conditions the isolate exhibited 85.10% degradation on 3rd day for the highly recalcitrant and less studied molecule. In simulating conditions, 76.78% of carbon was utilized from chrysene with $\pm$0.05 mg of carbon defeating on 18th day in validation experiment in microcosm system and almost all PAHs were degraded in crude oil spiked saline soil added in the microcosm flask. These results thus articulate the success story of bioremediation by the bacterial isolate *Achromobacter xylosoxidans* in polluted saline sites at Gujarat sea coast. This can be a driving force towards clean technology in making our oceans free of hazardous materials.

PP -297

Poster Presentations

Synthesis and production of poly (3-hydroxybutyrate) by halophiles

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ABSTRACT

Biodegradable materials with plastics or elastomeric properties are in great demand for a variety of applications. Polyhydroxyalkanoates (PHAs), polyesters synthesized by microorganisms possess such desirable features. Poly (3-hydroxybutyrate) (PHB) is the most common PHA stored in prokaryotes. Nevertheless, recent research on halophiles has shown a remarkable potential for biotechnological production of PHB. 13 halophilic Archaea were isolated from salt pans at Newport and Nari near Bhavnagar coast from which 12 isolates were non–alkaliphilic, while 1 was an alkaliphilic strain. Primary and screening data revealed that all the 13 isolates exhibited the ability to produce PHB–a thermostable biodegradable plastic. All the isolates were subjected to secondary screening for examining Dry cell weight, PHB production and PHB Yield as a function of incubation time. Maximum production of PHB was obtained by four isolates *Haloarcula* sp. 1, *Halorubrum* sp. 2, *Halobaculum* sp. and *Halobacterium salinarum* which were selected for further studies on PHB production and its chemical characterization. The effect of various cultural conditions, carbon and nitrogen sources (Natural and synthetic), phosphate limitation and various ratios of carbon:nitrogen on growth, PHB production and PHB yield had been examined in temporal sequence. Amongst these, *Haloarcula* sp. 1 showed maximum PHB yield (62%) within 8 days. As determined from various analytical techniques (^{1}H, ^{13}C-NMR, FT-IR, GC-MS, TGA and DSC) the bioplastic obtained was a polymer of monohydroxybutyrate. One of the enzyme i.e., â - Ketothiolase important in PHB synthetic pathway was optimized and purified from *Haloarcula* sp. 1. Thus halophiles hold promise for providing an economically competitive industrial scale production. Further research is needed to gain more extensive knowledge of the synthetic machinery and regulatory mechanisms controlling the polymer synthesis at the molecular level, which can be used for improving PHB production.

PP -298

Poster Presentations

QSAR/QSPR: Designing of new nonsteroidal anti-inflammatory drugs (NAISDs) considering diclofenac as a lead compound followed by selection of a good synthetic route through mathematical modeling

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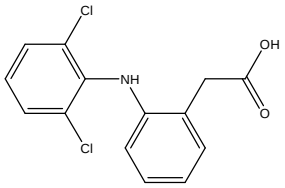
ABSTRACT

In this study new series of non steroidal Anti-inflammatory Drugs (NSAIDs) have been designed and their various physical properties and molecular descriptors [1] like log P, Dipole moment, Heat of formation, Ionization Potential, Wiener's index, HOMO (Highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) and pka were calculated by using several software such as Vega zz, Mopac, ADME and ChemDraw etc and compared with Diclofenac [2-6]. This paper focuses on the Quantitative structure activity relationship/Quantitative structure property relationship (QSAR/QSPR) [7] studies of series congeners of Diclofenac. The newly Designed compounds I&II having the comparable properties with that of Diclofenac are selected for their synthesis and by literature survey [8] various Retrosynthetic approaches can be considered and through mathematical modeling and by following Hendrickson equation [9] $W = ?\eta i X^{li}$, Where W = Sum of Weight, ηi - is number of skeletal carbons in each piece and X is reciprocal of the average yield for each step. The good synthetic route could be predicted.



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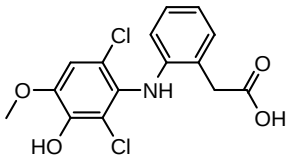

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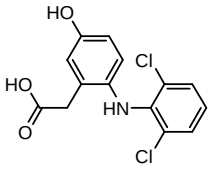

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PP -299

Poster Presentations

Multicomponent reaction (MCRs) as a green approach towards the synthesis of substituted pyridines

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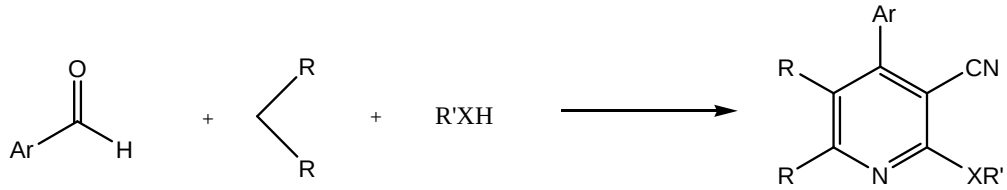
ABSTRACT

A facile and convenient synthesis of substituted pyridines has been developed *via* a one-pot multicomponent reaction[1] of easily available aromatic aldehydes, active methylene compounds and Phenols in the presence of solid base catalyst under mild conditions. A series of functionalized pyridines [2,3,4] were thus obtained. This protocol includes mild conditions, simple execution, broad substrate scope, and high yields of products which make it an efficient and promising synthetic strategy to build pyridine skeleton. The pyridine Skelton is one of the most prevalent heterocycle found in numerous natural and synthetic products with useful bio-, physico- and pharmacological activities [5].



Ar = Aromatic , HetAr R=CN,CH_3,$COOCH_2CH_3$ X= S,O

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PP -300

Poster Presentations

SAR: synthesis of new non steroidal anti-inflammatory drugs (NSAIDs) through selective halogenation

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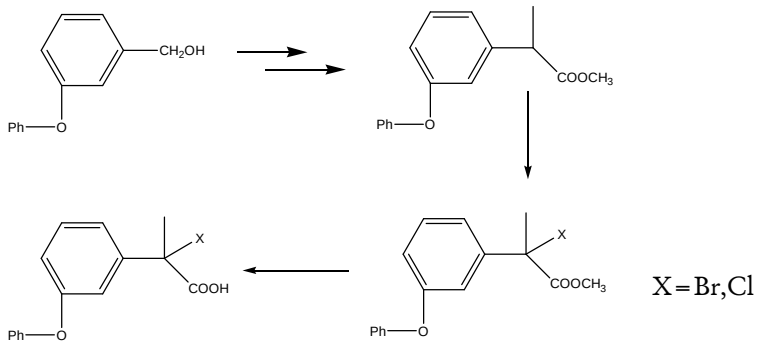
ABSTRACT

Structure-activity relationships (SAR) are the traditional practices of medicinal chemistry[1] which try to modify the effect or the potency (i.e. activity) of bioactive chemical compounds by modifying their chemical structure. Medicinal chemists use the techniques of chemical synthesis to insert new chemical groups into the biomedical compound and test the modifications for their biological effects. Fenoprofen is a nonsteroidal anti-inflammatory drug (NSAID) that is effective for treating the fever, pain, and swelling caused by inflammation. Other members of the NSAID class of drugs include Ibufrofen , Ketoprofen, Indomethacin (Indocin), Nabumetone (Relafen), Naproxen , Diclofenac and several others[2]. The Non steroidal anti –Inflammatory Drug can be prepared selective halogenation of Fenoprofen. The reaction is depicted in scheme 1 [3,4].



Scheme -1

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PP -301

Poster Presentations

Thermal profile and decomposition kinetics of some synthesized 1,5- benzodiazepines

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ABSTRACT

Thermal analysis of some 1,5-benzodiazepines derived from quinoline chalcones, have been carried out by TG and DSC technique. TG data of decomposition have been analysed for the kinetic parameters using Freeman-Carroll method. From the observed curves, various kinetic parameters such as order of degradation (n), energy of activation (E), frequency factor (A) and entropy change (?S) have been evaluated. Further, thermal stability of benzodiazepines have been determined, which is found to depend on the type of substituent present in the compounds.

PP -302

Saussurea oblovata, an endangered ethno-medicinal herb, possesses free radical scavenging activity

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ABSTRACT

Saussurea oblovata (Braham kamal; Asterceae) is an endangered medicinal herb found in upper Himalayas at an elevation of 3000-4500 m. It is found in alpine meadows, rocky slopes and along rivers in parts of Himacal Pradesh, Jammu and Kashmir, and Sikkim in India. It is traditionally used in Tibetan medicine system to treat limb paralysis. Roots are used to treat bruises and cuts, and seed oil is used against headache. However, no study has been conducted to explore its biological activity in terms of free radical scavenging. We investigated the antioxidant activity of dried *S. oblovata* plants against free radicals such as hydroxyl, nitric oxide, hydrogen peroxide, and superoxide anions. The water extracts (0.5–5.0 %, w/v) of the herb were found to scavenge hydroxyl and superoxide radicals and hydrogen peroxide in the range of 24 to 95%. Further, the extracts exhibited 28-83% DPPH radical scavenging activity. Upon investigation, the extracts were found to be rich in phenolics indicating their role in antioxidant activity of the herb. The present paper discusses the ethno-medicinal vis-à-vis antioxidant activity of the endangered herb *S. oblovata.*

PP -303

Poster Presentations

Synthesis, characterisation and biological activity of Fe (II), Co (II), Ni (II), Cu(II), Zn(II), Cd (II) and Hg(II) complexes of tridentate thiosemicarbazone Schiff base ligands

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ABSTRACT

Platinum based anticancer drugs induces normal tissue toxicity particularly to the kidneys and thus alternative metal compounds are presently being evaluated in clinical trials Transition metals are the most promising metals and are regarded as promising alternatives in cancer therapy and offer many approaches to innovative Metallopharmaceuticals.Thiosemicarbazones are a class of compounds whose biological activity is enhanced by the functional groups of the parent aldehyde or ketone.Solution chemistry, spectroscopic properities ,X-Ray structures and biological activity of different aromatic or aliphatic Thiosemicarbazones and their metal complexes have been studied for a long time.The real impetus towards developing the chemistry of these thiosemicarbazones has been provided by the remarkable biological properties observed for these compounds due to their metal complexation ability.In cancer treatment metal chelates are more potent than the chelating agents.

Metal complexes of divalent d-block metal ions with different thiosemicarbazones have been synthesized. These thiosemicarbazone ligands forms complexes with divalent metal ions such as iron (II), cobalt (II), nickel (II), copper (II), zinc (II), cadmium (II) and mercury (II). The present research reports the structural study of the complexes and have been characterised by elemental analysis, conductance, IR, NMR and Mass spectral data. The physico chemical and spectral data suggests octahedral and tetrahedrol geometry for various complexes. The ligand and metal chelates have been screened invitro for antimicrobial activity against some of the fungal and bacterial. The screening have revealed that metal complexes exhibit enhanced activity than their parent ligand – against both the fungal and bacterial strains used.These complexes are being tested for their anticancer activity as they are very good candidates as anticancer drugs.

PP -304

Poster Presentations

Au(III) and Ru(III)-benzil thiosemicarbazone complexes as potential anti-cancer drugs

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ABSTRACT

Inorganic chemotherapy has been considerably boosted in recent years by the discovery and exploitation of antitumor compounds based on platinum. Some Gold (III) complexes display similar chemistry and pharmacological activity to cis-platin and its analogues are now the basis of multimillion dollar industry and bring benefit to thousands of cancer patients.

Gold is one of the most promising metals and its compounds are regarded as promising alternatives in cancer therapy and offer many approaches to innovative Metallopharmaceuticals. Ruthenium is one of the most promising metals and its compounds are regarded as promising alternatives in cancer therapy and offer many approaches to innovative metallopharmaceuticals as these compounds are stable with predictable structures both in solid and solution states Thiosemicarbazones are a class of compounds whose biological activity is enhanced by the functional groups of the parent aldehyde or ketone.Solution chemistry, spectroscopic properities ,X-Ray structures and biological activity of different aromatic or aliphatic Thiosemicarbazones and their metal complexes have been studied for a long time.The real impetus towards developing the chemistry of these thiosemicarbazones has been provided by the remarkable biological properties observed for these compounds due to their metal complexation ability.In cancer treatment metal chelates are more potent than the chelating agents.

In this work we describe the synthesis and characterization of Gold (III) and Ru(III)-Benzil Thiosemicarbazone Complexes . A full range of gold(III) and Ruthenium(III)compounds have been synthesized and characterized and are currently being investigated for their potential as anti-tumor agents toward several human tumor cell lines and would be evaluated in-vitro using a systematic screening strategy for their utilization in cancer therapy. The structural features from the spectroscopic ie FT-IR,NMR,Magnetic and other studies qualify Gold(III) and Ruthenium(III) compounds as a promising class of cytotoxic agents of outstanding interest for cancer treatment.

PP -305

Poster Presentations

Synthesis and biological evaluation of some acetyl pyrazolines

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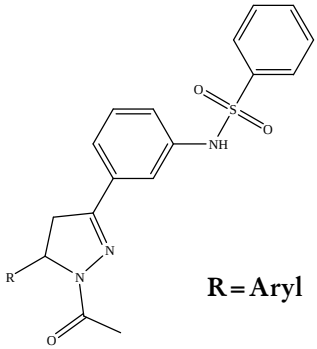
ABSTRACT

Amongst the heterocyclic compounds, nitrogen containing five membered heterocyclic compounds such as pyrazolines have been proved to the most active nucleus. Various substituted prazolines have specific applicability in the field of medicines and agriculture. Pyrazoline derivatives are associated with a wide range of biological activities like antidiabetic, antitumour, antileprosy, antitubercular, antibacterial, fungicidal, etc. In order to design better drug potentials and to study their pharmacological profile some 1-acetyl pyrazoline derivatives were synthesised.

Various 1-acetyl-3-(3'phenylsulphonamidophenyl)-5-aryl pyrazoline derivatives (Type-I) have been synthesised by the condensation of 1-(3'phenylsulphoamidophenyl)-3-aryl-2-propene-1-one with hydrazine hydrate in glacial acetic acid.

The constitution of the newly synthesised products have been confirmed by elemental analysis, IR, ^{1}H NMR spectroscopy and further supported by Mass Spectroscopy. The compounds have been evaluated for their antibacterial activity, against gram positive and gram negative strains of bacteria, and antifungal activity using cup-plate method at a concentration of 50 μg/ml. The antimicrobial activity was compared with standard drugs. It was observed that most of the compounds were found to be moderately active against different strains of bacteria and fungi.



R = Aryl

Type -I

PP -306

Poster Presentations

Fabrication of a cryo-ultrafine grinding machine for getting nano size medicinal plant material and its comparative study of safety and efficacy with normal particle size (85 mesh) material used in traditional indian medicines

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ABSTRACT

Traditional Indian Medicines have played an indispensable role in the prevention and treatment of diseases in India. The pharmacological effects of Traditional Indian Medicines are not only due to the special chemical components, but the form of dosage as well. The particle size of medicinal materials is an important physical property that affects pharmacological behaviors such as dissolution, chemical stability, and bioavailability of solid dosage forms. Nano size medicinal plant particles in modern medicine have proved to have enhanced efficacy. However very few reports on the efficacy of nano herbal medicines are available in literature.

In order to avoid deterioration of thermally labile phytoconstituents a special cryo-ultrafine grinding machine was fabricated. Plant nano particles thus obtained was characterized using SEM.

Comparative safety and efficacy studies of conventionally used 85 mesh plant powder and plant nano powder of Hiptage benghalensis bark were conducted for excision wound healing activity in rats. Plant nano powder exhibited comparable wound healing property with synthetic standard and ethanolic extract of plant bark but better wound healing property than the conventionally used 85 mesh particles.

PP -307

Poster Presentations

Studies on benzimidazole derivatives

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ABSTRACT

Several Benzimidazoles derivatives have found use in the preparation of Subburn Privantivrs. These compounds protect the skin by absorbing ultraviolet rays. Goodmann reported that benzimidazoles has a similar action on skeletal muscles. In addition to anticonvulsant activity and suggested that it might be of value in spastic condition and convulsine disorders. Benzimidazole shows anticonvulsant activity when administrated in rather large doses, Benzimidazole is relatively non toxic and has little effect on the blood pressure. Because of their relation to histamine a number of B-aminoethyl derivatives of benzimidazole have been studied 5 (or 6)-b-aminoethyl-benzimidazole or 2-methyl-5(or 6)-β-aminoethyl benzimidazoles are said to have a rise in blood pressure A large number of benzimidazole derivative are prepared and tested to show trypanosomicinal and spirothatical activity they are active against diseases caused by Protozoa.

PP -308

Synthesis of Dihydropyrimidines via Green Chemistry routes

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ABSTRACT

Dihydropyrimidinones have good pharmacological properties. They are prepared by various methods but the classic method for their synthesis is Biginelli Reaction or Condensation. The acid-catalyzed, three-component reaction between an aldehyde, α,ß-ketoester and urea constitutes a rapid and facile synthesis of Dihydropyrimidinones . This is known as Biginelli Reaction. This can be done by taking either different reagent or by taking different starting material in presence of various catalysts. Green Chemistry route is Dihydropyrimidinones can be synthesized with the help of arsenious acid solution (H_3AsO_3 / $AsCl_3$) as catalyst under microwave irradiation in 6 -7 minutes.

But all methods have some drawback to overcome these problems here we have presented One of the simplest green method to synthesize Dihydropyrimidinones is via 'Grindstone Chemistry'.

PP -309

Poster Presentations

Synthetic and pharmacological studies on dichotomin A

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ABSTRACT

Dichotomin A is a natural cyclic hexapeptide which is isolated from the roots of Stellaria dichotoma L. var. lanceolata Bge (Caryophyllaceae) [1]. Keeping in view the biopotential of cyclopolypeptides from higher plants [2] and to obtain a bioactive cyclooligopeptide in good yield, the present study was directed toward synthesis of dichotomin A by solution-phase technique of peptide synthesis [3].

In order to carry out the synthesis, the peptide molecule was disconnected into two dipeptide units Boc-L-Thr-L-Phe-OMe **1**, Boc-L-Tyr-L-Val-OMe **2** and two amino acid units L-Leu-OMe.HCl **3** and Gly-OMe.HCl **4**. Dipeptide **1**, after deprotection at carboxyl terminal by esterification, was coupled with amino acid methyl ester hydrochloride **3** to get the tripeptide Boc-L-Thr-L-Phe-L-Leu-OMe **5** which was further deprotected at carboxyl terminal by alkaline hydrolysis with LiOH. Similarly, dipeptide **2**, after deprotection at carboxyl terminal was coupled with amino acid methyl ester hydrochloride **4** to get other tripeptide Boc-L-Tyr-L-Val-Gly-OMe **6**, The tripeptide **6**, after deprotection at amino terminal, was coupled with deprotected tripeptide unit **5** deprotected at carboxyl end, using diisopropylcarbodiimide (DIPC) and triethylamine (TEA) to get linear hexapeptide unit Boc-L-Thr-L-Phe-L-Leu-L-Tyr-L-Val-Gly-OMe **7** which was finally cyclized in presence of pyridine to get dichotomin A **7**. The structure of synthesized peptide was elucidated by spectral as well as elemental analysis. The newly synthesized cyclopeptide was found to possess potent antifungal activity against dermatophytes and pathogenic Candida albicans. In addition, moderate antibacterial activity against gram-negative bacteria was observed for synthesized cyclooligopeptide [4].

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PP -310

Poster Presentations

1, 3, 5-Substituted triazine: an efficient fluorescent probe for protein bioconjugation

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ABSTRACT

Fluorescent triazines have wide application in the field of biology as probe molecules for biomedical diagnostics and bioinformatics. They also find application in forensic, military, online monitoring of bioprocess, high-tech application, industrial and environmental monitoring. Interactions of probe molecule with biological system are subject of interest in biomedical diagnostics and bioinformatics [1]. Study of physico-chemical interactions within biological systems is interesting for chemists and biologists to understand the secret of life. These interactions are useful in clinical diagnosis and theranostics. These principles are also of importance in environmental monitoring, online monitoring of bioprocesses, and immunology-based sensing. Since radiological techniques are considered harmful fluorescent molecules are gaining importance as molecular probes. Organic fluorophores however suffer from lower photophysical and photochemical stability, short fluorescence lifetime and low fluorescent quantum yield in the biological microenvironment [2]. To overcome these limitations it is necessary to develop novel fluorescent probe molecules which have high fluorescent lifetime, high photo stability, and appreciably higher fluorescence quantum yield.

In the present study various novel fluorescent molecules which can function as molecular probes on bioconjugation are designed and synthesized from substituted triazine. The photophysical properties of fluorescent molecules as well as their bioconjugates like absorption emission characteristics and fluorescent quantum yield are reported. Proposed molecule is shown in figure.

The novel fluorescent molecules which function as recognition elements in the probes are confirmed by FT-IR, ^{1}H NMR and mass spectral analysis. Photo–physical and thermal studies were done by UV-Vis. Spectrofluorometer and thermo gravimetric analysis. The bioconjugation was carried our using the protein, bovine serum albumin.

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PP-311

Poster Presentations

7, 9-Disubstituted fluoroscein: fluoroscent porbes for covalent bioconjugation with protein

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ABSTRACT

Fluorescent molecules are gaining interest in recent years because of their extensive use as recognition elements as sensors for the detection of different antigenic cells in diagnostic and theranostic applications [1]. Detecting and tracing speci?c bio receptor molecules of interest are important for studying the function and the behaviour of biological systems. However, the available molecules suffer from limitations like short fluorescence lifetime, low photo stability in the biological microenvironment, and low fluorescent quantum efficiency of the bio conjugates [2].

In this paper we report novel fluorescent molecules which can function as molecular probes on bioconjugation. They are synthesized from substituted benzimidazoles, benzoxazoles and benzthiazoles. The photophysical properties of fluorescent molecules as well as their bioconjugates like absorption emission characteristics and fluorescent quantum yield are reported.

The novel fluorescent molecules which function as recognition elements in the probes are confirmed by FT-IR, ^{1}H NMR and mass spectral analysis. Photo–physical and thermal studies were done by UV-Vis. Spectrofluorometer and thermogravimetric analysis. The bioconguation was carried our using the protein, bovine serum albumin.

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PP -312

Poster Presentations

Pd/C: an efficient, heterogeneous and reusable catalyst for phosphine-free carbonylative Suzuki coupling reactions of aryl and heteroaryl iodides

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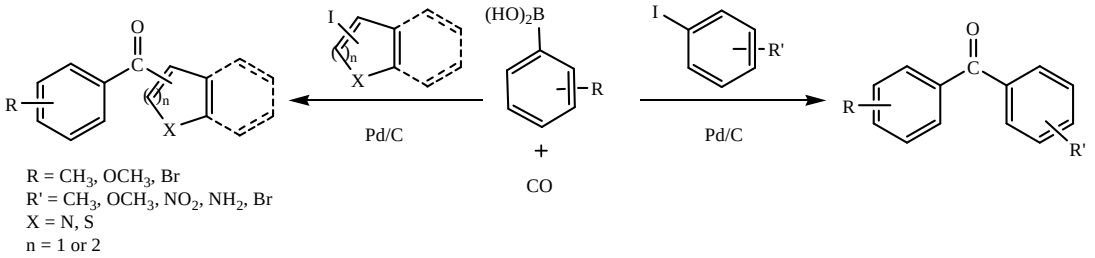
ABSTRACT

Synthesis of biaryl and heteroaryl carbonyl compounds has attracted considerable interest, as they are important building blocks for various natural products, biologically active compounds and pharmaceutical compounds. In 1993, Suzuki et al. reported a facile protocol for the synthesis of biaryl ketones from carbon monoxide, aryl halide and aryl boronic acid by using palladium catalyst (1), Various palladium based catalytic systems have been developed, however reported methods suffer from one or more drawbacks. Therefore, the search for a heterogeneous and reusable catalyst that could efficiently catalyze the carbonylative Suzuki coupling reaction without the aid of phosphine ligands is the subject of the present work.

So the present work demonstrates an efficient, heterogeneous and reusable catalytic system for the carbonylative Suzuki coupling reaction of aryl and heteroaryl iodides with various aryl boronic acids. The present protocol affords good to excellent yield of desired products and demonstrating the broad application of the methodology. Catalyst reusability and Pd leaching were also examined and Pd/C effectively recyclable for four consecutive cycles without any significant loss in catalytic activity.



Scheme 1. Carbonylative Suzuki coupling reaction.

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PP -313

Poster Presentations

Allylic amination of internal alkynes with aromatic and aliphatic amines using polymer-supported triphenylphoshine palladium complex as a heterogeneous and recyclable catalyst

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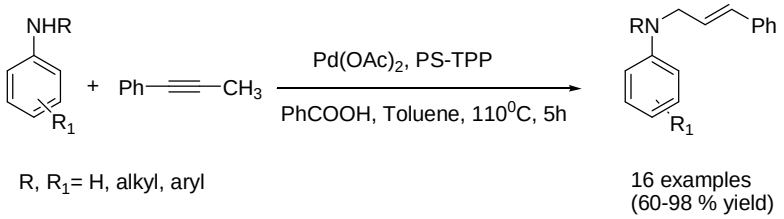
ABSTRACT

Allylamines are very important organic compounds due to their wide applications as intermediates in organic synthesis, biological properties, and their existence in several natural products. Synthesis of these allylamines by allylic amination of alkynes is much more efficient and greener as compared to synthesis using allylic amination of allylic alcohols and their derivetives. As the products of allylic amination of alkynes were obtained through formal addition of amines to alkynes, no waste was produced after completion of the reaction. allylic amination by using homogeneous palladium complexes produces palladium-based waste products in the reaction and lacks catalyst recyclability.

The present work demonstrated a facile and novel protocol for allylic amination of internal alkyne with various amines using polymer-supported triphenylphosphine-palladium complex [PS-TPP-Pd] as highly active heterogeneous reusable catalyst. The reaction is optimized with respect to solvent, temperature, time, catalyst loading and metal:ligand ratio ($Pd(OAc)_2$:PS-TPP). The catalyst exhibited remarkable activity and is reusable for five consecutive cycles. The methodology offers a first heterogeneous and recyclable catalyst system which was applicable for variety of hindered and functionalized aromatic/aliphatic amines. The present protocol afforded the desired allylic products in good to excellent yield (60-98 %).



Scheme 1. Allylic amination of internal alkyne with aliphatic/aromatic amines.

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PP -314

Poster Presentations

Development and validation of eight antihypertensive drugs in pharmaceutical products by UPLC-PDA

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ABSTRACT

An UPLC-PDA method was developed and validated for the simultaneous quantitative determination of diltiazem, quinapril, Valsartan , candesartan, carvedilol, olmesartan, ranolazine and Losartan for the determination of compounds in pharmaceutical products. The separation was achieved on Acquity UPLC BEH C8 (100mm X 2.1mm, 1.7μm, Waters) column by use of a mobile phase consisting of 0.2% Formic acid aqueous solution and acetonitrile 13 min. All calibration curves were linear (R^2=0.9990) over the tested ranges. The linearity ranges were 42.56 to 191.52 μgmL^{-1} for diltiazem, 40.64 to 182.88 μgmL^{-1} for quinapril, 41.92 to 188.64 μgmL^{-1} for Valsartan, 40.00 to 180.00 μgmL^{-1} for candesartan, 40.32 to 181.44 μgmL^{-1} for carvedilol, 44.16 to 198.72 μgmL^{-1} for olmesartan, 40.96 to 184.32 μgmL^{-1} for ranolazine and 43.20 to 194.40 μgmL^{-1} for Losartan. The method was validated by

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Poster Presentations

Synthesis and anti-bacterial activity of poly-substituted pyrrole derivatives

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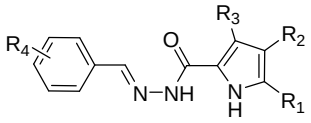
ABSTRACT

Organic compounds possessing nitrogen containing five membered heterocyclic rings are widely distributed in nature and often play an important role in various biochemical processes. Nitrogen containing heterocycles are subunits found in numerous natural products and in many biological active pharmaceuticals. Therefore, here in we have reported easy and efficient synthesis of poly-substituted pyrrole via condensation of α-amino β-keto esters with acetyl acetone and their anti-bacterial activity.



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Cultivation of Some important Medicinal important plants and their production at Implant, Saurashtra University, Rajkot

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ABSTRACT

Medicinally importnat *Aloe barbadensis* (Aloe vera) and *Senna alexendrina* (Senna) were cultivated as intercrop with *Moringa oleifera* (Drum stick) at IMPLANT, Saurashtra University, Rajkot. The biomass production of various part of the plant i.e., leaves; roots, fruits (pod, husk, seeds) and other essential parts of the plants were studied and documented. The cultivation was found to be economically feasible for poor/waste lands.

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Poster Presentations

Study of New Homologous series of Azoester Mesogens: p-(p'-n-alkoxybenzoyloxy)-m-methylphenylazo-p''-methoxybenzene

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ABSTRACT

A new homologous series of azoester mesogens: p-(p'-n-alkoxybenzoyloxy)-m-meyhyl phenylazo-p''-methoxybenzenes has been synthesized with a view to understand the relation between liquid crystal preparation and molecular structure. Transition temperatures of the members of the homologous series are observed under Leits Labourlux 12 POL-polarizing microscope with heating stage. The homologues of the series show variation in textures and transition temperatures. Mesomorphism commences from the very first homologue of the series. All the members of the series exhibit enantiotropic mesomorphism except third member which exhibit monotropic-nematic behavior. Smectic mesophase commences from the dodecyl homologue of the series. Dodecyl homologue of the series exhibit polymesomorphism i.e. smectic and nematic phase are present, one after another. The series is of high melting type with considerable mesomorphic range. The thermal stabilities and mesomorphic properties of the series have been compared with other structurally similar homologous series. Texture of the nematic mesophase is of threaded type and that of smectic mesophase is, focal conical fan shaped of type- A for dodecyl and tetradecyl homologue and smectic-C for hexadecyl homologue as determined by miscibility method. Analytical data support the structure of molecules.

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