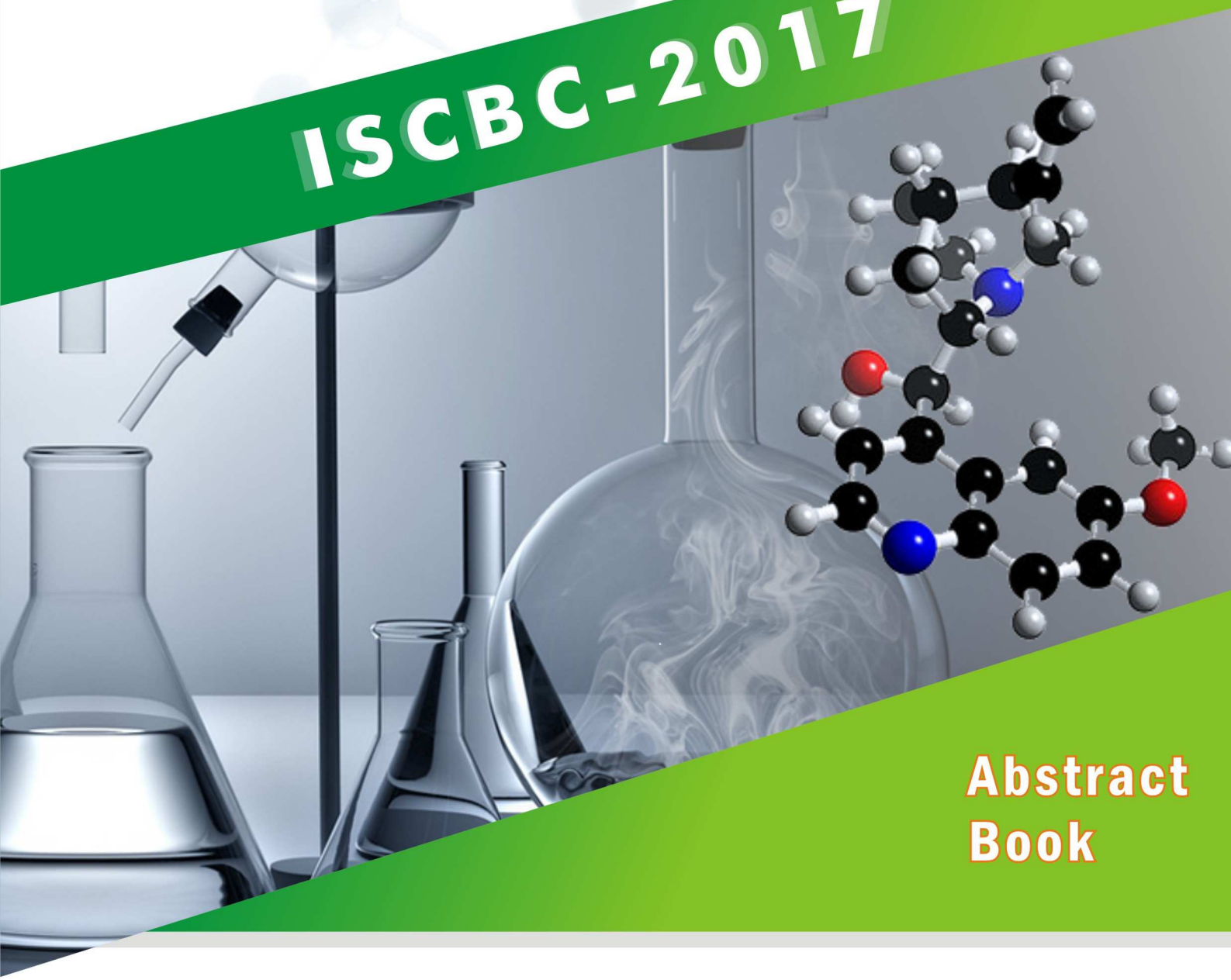
SRM UNIVERSITY
(Under section 3 of UGC Act 1956)

# ISCBC-2017



## Abstract Book

# 23rd ISCB International Conference

8-10 February 2017
at
SRM University, Chennai, India

## Interface of Chemical Biology in Drug Research

Jointly Organized by:
Indian Society of Chemists & Biologists, India
SRM University, Chennai, India

www.iscbindia.com

**Sponsored by:**

- SRM University
- Indian Council of Medical Research (ICMR)
- Department of Science & Technology (DST)
- SciFinder
- Southernindia Scientific Corporation
- Dr. Reddy's Laboratories, Hyderabad

**Prof. Anamik Shah**
President, ISCB

**Dr. P.M.S. Chauhan**
General Secretary, ISCB

## Message

Interdisciplinary interactions of researchers are of prime importance for the advancement of knowledge and applications of knowledge. Such interactions are much more important when come to drug research. However the process of drug research has become more difficult, risky and expensive due to very tight regulatory parameters. To make a breakthrough in this area a close interaction between the scientist and technologists in the area of chemistry and biology is highly desired. With this view in mind **Indian of Society Chemists and Biologists** is making consistent efforts to encourage interdisciplinary research activities in the field of chemistry and biology. **Indian Society of Chemists and Biologists** is unique in the sense that it promotes multidisciplinary research as compared to several scientific societies in the individual capacity with confined objectives. During the past the society has been very successful in achieving the targets. We are extremely happy that With great Pleasure, Indian Society of Chemists and Biologists (www.iscbindia.com) organising its 23rd ISCB International Conference (ISCBC-2017) on "Interface of Chemical Biology in Drug Research" from 8th-10th February, 2017 at SRM University, Chennai.

ISCB conference has prime objective to provide an opportunity for a close interaction of scientists with varied interests in diverse fields of the research. Conference will also provide common platform and more opportunities to the researchers in the areas of chemical sciences and biological sciences and other related areas to interact with each other. ISCBC will also provide a forum for in-depth assessment of the challenges involved in the dynamic and fast moving field of Drug research. It will bring together leading Chemists, medicinal chemists, pharmacologists, biotechnologists, and other allied professionals to discuss and present the latest important developments in drug discovery and therapeutics. It is expected that approximately 600 delegates will participate coming from different part of India and abroad. A large number of pharmaceutical and biotechnology industry professionals will join us for this event, share ideas and built networks.

I take this opportunity to express my sincere thanks and gratitude to members and office bearers of the society without their untiring efforts we would have not reached the present stage. We are glad that the scientific committee is bringing out an abstracts book covering the presentation to be made during 23rd ISCB International Conference (ISCBC-2017) of Indian Society Chemists and Biologists (ISCBC-2017). Our sincere

thanks are due to the members of scientific committee. During this conference a number of eminent scientists and technologists of the country and abroad will be discussing the trends, prospects and future directions of research. We look forward to fruitful deliberations in extremely interesting areas of scientific research. We are happy that an extensive and comprehensive scientific program is arranged. The scientific program beside inaugural function includes 13 plenary lectures, 25 invited lectures by the eminent scientists and 40oral presentations by the young researchers are scheduled. The most heartening feature of the conference is that it is being participated with a number of young scientists and Ph. D. students and more than 250 poster presentations are schedules for two different poster sessions. ISCB has achieved a prominent status in its 23rd international conference. We are looking to the galaxy of speakers and young participants who made this conference a memorable and international event. We extend our warm welcome to all national and international delegates from pharmaceutical companies, research organization, universities and academic institutes wish them very happy stay at SRM, Chennai .

**(Prof. Anamik Shah)**
President, ISCB

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

SRM UNIVERSITY
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Date: 21.01.2017

**Dr. T .R. Paari Vendhar**
Founder Chancellor

## Message

It is a great pleasure for me to welcome all the delegates, speakers from the whole area of the country and abroad to the 23rd ISCB International Conference with the theme of "Interface of Chemical Biology in Drug Research", from 8th to 10th February, 2017 at SRM University

Indian Society of Chemists and Biologists (ISCB) has evolved into one of the most important organization has made a substantial contribution throughout India dedicated to research in the basic subjects of chemistry and biology towards drug discovery and development.

ISCB in co-operation with the worldwide scientists of chemistry and biology has involved with most appropriate themes on Drug Research, Chemical Sciences, Bionanotechnology, Chemical Biology, and Biochemistry which helps to establish the unanimity of their knowledge skills in drug discovery.

I am sure that this conference would be a wonderful platform for the Pharmaceutical fraternity as well as the scholars of other disciplines both from India and abroad, to interact and work out a future strategy. I hope that this conference helps the academicians get exposed to the latest development in their respective fields.

My warm greetings and best wishes to all the delegates and participants. I would like to congratulate the organizers involved in conducting the conference.

T. R. Paari

Founder Chancellor

SRM UNIVERSITY
(Under section 3 of UGC Act 1956)

Date: 21.01.2017

**Mr. Ravi Pachamoothoo**
Chairman,
SRM Institute of Science & Technology

## Message

It is an immense pleasure that our College of Pharmacy, SRM University, is organizing the 23rd ISCB International Conference with the theme of "Interface of Chemical Biology in Drug Research'' from 8th to 10th February, 2017 at SRM University.

The conference will provide a great platform for the scientists and young scholars to discuss and present the recent important developments in the arena of their research towards drug discovery and therapeutics.

We would like to extend our warm welcome to all the National and International delegates from various pharmaceutical companies, research organizations, academic institutes and universities for the conference. At the same time I wish the scientists and delegates a very happy and comfortable stay at Chennai.

Finally I take this opportunity to express my sincere thanks and gratitude to all members and office bearers of organizing committee of 23rd International Conference (ISCBC-2017) for conducting this conference at SRM University.

I WISH THE CONFERENCE A GREAT SUCCESS.

Chairman

SRM UNIVERSITY
(Under section 3 of UGC Act 1956)

Date: 21.01.2017

**Dr. P. Sathyanarayanan**
President

## Message

I am happy to note that the College of Pharmacy, SRM University and ISCB Lucknow are jointly organizing the 23rd International Conference on "Interface of Chemical Biology in Drug Research" from 8th to 10th February, 2017 at SRM University.

I feel it would be an ideal forum to bring together the world class chemists, pharmacologists, biotechnologists, and other professionals from different parts of India and abroad to share their views and opinion on the recent trends for incorporating chemical biology in the field of drug research.

In addition I am sure it would be a very good learning experience for students, researchers, academicians and industrialists. My best wishes to the members of Indian Society of Chemists and Biologists, the local organizing committee and all participants to have a very successful conference.

President

SRM UNIVERSITY
(Under section 3 of UGC Act 1956)

Date: 21.01.2017

**Dr. R. Sivakumar**, M.D., Ph.D.,
Vice-President, SRM University

## Message

It indeed gives me a sense of pride in welcoming all the eminent scientists and young researchers both from the nation and world-wide for the 23rd ISCB International Conference on "Interface of Chemical Biology in Drug Research" from 8th to 10th February, 2017 at SRM University.

The field of chemical biology and drug research is currently witnessing a renaissance in drug discovery and development process. This chemistry, biology, medicine continuum of research in academia will translate into new opportunities and paradigms in biological pathways and disease pathogenesis which are efficient, productive and profitable.

ISCB comprises a team of expert scientists, technologists and entrepreneurs as members who have an open vision of sharing their fruitful research experiences and cultivate collaborative research across the world. The members, through their research and strategic collaborations are focused to solve newly defined challenges and exploit the opportunities in this field.

I am confident that this conference will provide a perfect venue for close interactions and exchanges among the participants in this transdisciplinary arena, thus paving the way for new innovations in drug design and discovery.

I wish all the delegates and speakers a pleasant and productive experience during the conference. I am sure that this conference would definitely induce very fruitful and rewarding cutting edge ideas among the participants.

My hearty congratulations to the organizing committee for their constant and continuous efforts. I extend my warm greetings and felicitations to the participants.

R. Sivakumar

Vice President

SRM UNIVERSITY
(Under section 3 of UGC Act 1956)

Date: 21.01.2017

**Professor PRABIR K. BAGCHI,** B.E., M.S., Ph.D.(Tenn., USA)
Vice Chancellor

## Message

Dear Organizers,

The theme of the conference, "Interface of Chemical Biology in Drug Research" has become appropriate in the contemporary field bringing together the pharmaceutical fraternity with basic and applied sciences. At this conference, a collaborative knowledge exchange between researchers in chemistry and biology can help immensely in expediting purposeful research for finding cures for interactable diseases. I am sure that the conference will provide the right platform to establish a network among researchers from various institutions in the country and lead to new innovative strategies for drug development.

I WISH THE CONFERENCE A GRAND SUCCESS.

Best Regards.

Vice Chancellor

SRM UNIVERSITY
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Date: 21.01.2017

**Dr. T.P. Ganesan**
**Pro Vice Chancellor** (P&D)

## Message

It is my great pleasure to welcome you all whole heartedly to the 23rd International Conference on "Interface of Chemical Biology in Drug Research", from 8th to 10th February, 2017 at SRM University.

ISCB has established itself as a worldwide reference for the dissemination of high-quality research projects, process developments, information regarding IPR and patent writing, quality control etc and for fostering interaction and exchange of ideas for the past two decades.

I have full hope that the conference is going to be informative besides intellectually stimulating, with eminent speakers from all over the country and abroad to discuss on the contemporary fields of medical research.

I welcome and applaud the ISCB conference 2017 a note worthy event among the various events conducted in SRM University. I pray God to shower blessing to the organizing committee for their dedication and hard work to bring this conference to great heights.

I WISH THE CONFERENCE A TREMENDOUS SUCCESS.

T.P. Ganesan
18.1.17

Pro Vice Chancellor (P&D)

SRM UNIVERSITY
(Under section 3 of UGC Act 1956)

Date: 21.01.2017

**Prof. Dr. P. Thangaraju,** Ph.D.,
Pro Vice Chancellor (Medical)

## Message

I am pleased to know that SRM College of Pharmacy is organizing the 23rd ISCB International Conference with the theme of "Interface of Chemical Biology in Drug Research" a creative way to explore the future from 8th to 10th February, 2017 at SRM University.

Today technology and research is developing at a very faster pace. We all know that our country can make a progress if the scientist and technocrats utilize their knowledge for exploring newer fields in the area of biological research and development. It is rightly sensed that ISCB is going to provide a wide platform for all the researchers round the globe to bring forward their thoughts and to help our pharmacy society at large.

My warm greetings and hearty welcome to all the speakers and participants of this conference. I congratulate the organizers for organizing this conference on a topic of growing importance.

I WISH THE EVENT A GRAND SUCCESS.

21.1.17.

Pro Vice Chancellor (Medical)

SRM UNIVERSITY
(Under section 3 of UGC Act 1956)

Date: 21.01.2017

**Prof. N. Sethuraman,** M.A., M.Phil., Ph.D.
Registrar

## Message

It gives me a great pleasure to welcome you all to the 23rd ISCB International Conference with the theme on "Interface of Chemical Biology in Drug Research" from 8th to 10th February, 2017 at SRM University.

The overwhelming response to our call for papers indicates the popularity of this conference and confirms that ISCB has become the world wide forum for all aspects of Biology and Chemistry in the field of Drug Research related topics. The enthusiasm has certainly increased due to the successful organization of symposia, conferences and special lectures in various disciplines of drug development for the past two decades.

I wish all the organizers my best wishes and hearty congratulations for their strenuous and patient efforts to make this conference a grand success.

Registrar

SRM UNIVERSITY
(Under section 3 of UGC Act 1956)

Date: 21.01.2017

**Dr. N. Chandraprabha,** M.D., D.A.
Director - Health Sciences

## Message

I am pleased to understand that the 23rd ISCB International Conference (ISCBC-2017) is jointly organized by ISCB and SRM College of Pharmacy, SRM University on "Interface of Chemical Biology in Drug Research" scheduled to be held from 8th to 10th February, 2017at SRM University, Chennai.

We feel proud to conduct this conference for the first time in Southern Part of India. This forum comprises of Academicians, Scientists, Technologists, Chemists, Biologists, Pharmacist and Industrialists, who will be sharing their expertise and ideas.

This conference will provide lot of opportunity for multidisciplinary research, promote awareness of recent advances and developments in areas of science and help to organize symposia, conferences and special lectures in various disciplines of science. I am sure this is going to be a great academic fest for the participants, who can get benefited with the deliberations of eminent speakers.

31 National and 18 International speakers will be exchanging their ideas and sharing their experiences in various fields.

I congratulate the organizers and convey my best wishes for success of this conference.

Director - Health Sciences

SRM UNIVERSITY
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Date: 21.01.2017

**Dr. James Pandian,** M.S., M.Ch.,
Director ( Medical)

## Message

I am very happy to note that the 23rd ISCB International Conference (ISCBC-2017) is hosted in SRM University Campus, Chennai. All systems of medicine and health services are based upon proper drug identification, distribution and scientifically planned administration. Lot of avenues are available for researchers to find out appropriate, less harmful drugs for so many diseases. All allied biological departments, if they are utilized properly with thoughts and innovative ideas, we may claim up the ladder in research very well. Hence, I feel the utility of the conference deliberation, will pave way for better drug research and human health care delivery systems.

I WISH THE CONFERENCE A GRAND SUCCESS.

Director - Health Sciences

SRM UNIVERSITY
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Date: 21.01.2017

**Dr. A. Sundaram**
Dean ( Medical)

## Message

It is a great pleasure and an honour to extend you a warm invitation to all participants to attend the 23rd ISCB International Conference, with the theme on "Interface of Chemical Biology in Drug Research"from 8th to 10th February, 2017 at SRM University.

The Conference will feature a highly interactive, stimulating and multidisciplinary program including plenary sessions as well as oral abstract and poster presentations. ISCB 2017 will address the entire pathway of collaborative research with chemistry and biology which attracts young minds of research toward drug discovery. The Conference will also provide the ideal forum to stimulate ideas and novel scientific thoughts in both the fields of research for drug discovery.

I WISH THE CONFERENCE A GRAND SUCCESS.

Dean (Medical)

SRM UNIVERSITY
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Date: 21.01.2017

**Dr. K.S. Lakshmi,** M.Pharm. Ph.D.,
Organizing Secretary

## Message

On behalf of the SRM College of Pharmacy, SRM University, Kattankulathur, I would like to express our warmest invitation to all National and International speakers and delegates from nationwide to the 23rd ISCB International Conference (ISCBC-2017), the theme of the conference entitled "Interface of Chemical Biology in Drug Research", which is scheduled from 8th to 10th February, 2017 at SRM University.

The ISCB has been organizing the conference for the past 22 years and this year it is being organized at SRM College of Pharmacy, SRM University. This conference will surely confront diverse ideas in the field of drug discovery, which is a great challenge for this generation research scientists broadly towards drug design.

The theme of the conference has been chosen to reflect on new drug discovery for the ultimate benefit of the society. The program of this conference includes valuable scientific sessions both by International and National scientists and eminent chairpersons and posters presentation which would motivate young researchers.

I sincerely express my indebted gratitude to our Honourable Chancellor Dr. T. R. Paarivendhar; Honourable Chairman Mr. Ravi Pachamoothoo; Honourable President Dr. P. Satyanarayanan; Honourable Vice President Dr. R. Shivakumar; Hourable Vice Chancellor Prof. Prabir K. Bagchi; and our most respected Pro Vice Chancellor (P&D) Dr. T.P. Ganesan; and Pro Vice Chancellor (Medical) Dr. P. Thangaraju; Registrar Dr. N. Sethuraman, Director, (Health Sciences) Dr. N. Chandraprabha; for their constant support to organize this scientific event at this reputed university.

My hearty congratulations to the prominent resource persons from reputable foreign and Indian universities who are expected to share their proficiencies in their areas of concern. It will be a grand platform for the best of minds to meet deliberate and envision a greater commitment to the future of drug research. At this auspicious moment, I am very much glad to appreciate my staff members, who have taken a strong initiative to organize such a conference in collaboration with ISCB.

I WISH THE CONFERENCE A GRAND SUCCESS.

Organizing Secretary

## International Advisory Board ISCBC-2017

**Prof. Jyoti Chattopadhyaya,** Chair of Chemical Biology, Uppsala University, Uppsala, **Sweden**
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**Dr. K. S. Lakshmi**, Dean, SRM College of Pharmacy, SRM University, India

**Organizing Members:**
Dr. V. Chitra

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|---|---|
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**23rd ISCB International Conference (ISCBC-2017)**

**Interface of Chemical Biology in Drug Research**

**February 8-10, 2017**

**Jointly Organized by**
**Indian Society of Chemists & Biologists, Lucknow, India**
**SRM University, Chennai, India**
**at**
**SRM University, Chennai, India**

## PRELIMINARY SCIENTIFIC PROGRAMME

**Wednesday, February 8, 2017**

| | | |
|---|---|---|
| 9.00 AM - 10.30 AM | **Registration** | |
| 10.30 AM - 12.00 PM | **Inaugural Session** | |
| 10:30AM | Arrival of Guests | |
| 10:35AM | Deep Pragatya and Ganesh Vandana and Floral Welcome | |
| 10:40AM | Welcome Address | |
| 10:50AM | Introduction to ISCB | **Dr. P.M.S. Chauhan, Gen. Secretary ISCB** |
| 11:00AM | Presidential Address | **Prof. Anamik Shah** |
| 11:10AM | Provost Address | |
| 11:15AM | ISCB Award Distribution | |
| 11:30AM | Address by Chief Guest | |
| 11:35AM | Address by Guest of Honour | |
| 11:45AM | Keynote Lecture | |
| 12:15PM | Vote of Thanks | |
| **12.15 PM - 12.30 PM** | **High Tea** | |

**Session – I**

**Chairperson: Prof. Erik V. Van der Eycken**

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|---|---|
| **PL-1**<br>12.30 PM - 1.00 PM | **Kevin H. Shaughnessy**<br>Department of Chemistry, The University of Alabama, Tuscaloosa, AL 35487, USA<br>**UNRAVELING THE IMPACT OF LIGAND STERIC ELECTRONIC PROPERTIES ON METAL-CATALYZED BOND-FORMING REACTIONS** |
| **1.00 PM - 2.00 PM** | **Lunch** |
| **ISCB Award Lectures**<br>2.00 PM - 2.20 PM | **Michael D. Threadgill (ISCB Excellence Award 2017)**<br>Drug & Target Discovery, Department of Pharmacy & Pharmacology, University of Bath, Claverton Down, Bath BA2 7AY, UK<br>**Extreme potency and selectivity in the design of inhibitors of the tankyrases, new targets in cancer and other diseases** |
| 2.20 PM - 2.40 PM | **Ayyappanpillai Ajayaghosh (ISCB Excellence Award 2017)**<br>Director, CSIR-National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), Industrial Estate PO, Pappanamcode, Trivandrum, India<br>**Fluorescent Molecules in Sensing and Imaging of Bio-analytes** |
| 2.40 PM - 2.50 PM | **Ravi Prakash Singh (ISCB Young Scientist Award 2017)**<br>Assistant Professor, Indian Institute of Technology (IIT Delhi), New Delhi, India<br>**Development in selective C-C bond formation: From Asymmetric Catalysis to C-H activation** |
| 2.50 PM - 3.00 PM | **P. Anbarasan (ISCB Young Scientist Award 2017)**<br>Associate Professor, Indian Institute of Technology (IIT Chennai), Chennai, India<br>**Rhodium Catalyzed Transannulation of *N*-Sulfonyl-1,2,3-Triazoles** |
| 3.00 PM - 3.10 PM | **Amit Mishra (ISCB Young Scientist Award 2017)**<br>Associate Professor, Indian Institute of Technology (IIT Jodhpur), Jodhpur, India<br>**Proteostasis Restoring Factors: Molecular StrategiesAgainst Neurodegeneration and Ageing** |
| 3.20 PM - 3.35 PM | **Farukh Arjmand (Distinguish Women Scientist Award 2016)**<br>Department of Chemistry, Aligarh Muslim University, Aligarh 202002, Uttar Pradesh, India<br>**De novo tailored design of new metal-based drugs or drug precursors for antitumor chemotherapy: Structure elucidation by Single X-ray crystallography and their *in vitro* binding and cytotoxicity profile** |
| 3.35 PM - 3.55PM | **M. S. Shingare (ISCB Life Time Achievement Award 2017)**<br>Emeritus Scientist, CSIR, Dr. Babasaheb Bhimrao Ambedkar University, Aurangabad, India<br>**HIGHLY EFFICIENT SYNTHETIC STRATEGIES FOR BIOACTIVE HETEROCYCLIC MOLECULES** |
| 3.55 PM - 4.25 PM | **Tea** |

**Parallel Session – II A**

**Chairpersons: Dr. M.Vairamani and Dr. Vikas Shreekrishna Shirsath**

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|---|---|
| **PL-2**<br>4.30 PM - 5.00 PM | **Mahesh K. Lakshman**<br>Department of Chemistry and Biochemistry, The City College of New York, 160 Convent Avenue, New York, New York 10031, USA<br>**A Novel Approach to C6 Benzotriazolyl Purine Nucleoside Analogues** |
| **IL-1**<br>5.00 PM -5.20 PM | **Arun K. Sinha**<br>Medicinal and Process Chemistry Division, C.S.I.R- Central Drug Research Institute, Sector 10, Janakipuram Extension, Sitapur Road , Lucknow 226021, India<br>**Natural and Unnatural Phenolic Based Small Molecules: Green Chemical Synthesis and their Biological Evaluation** |
| **IL-2**<br>5.20 PM - 5.40 PM | **Bapurao B. Shingate**<br>Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431 004, Maharashtra, India<br>**A Small Focused Library of Diversely Functionalized Biodynamic Heterocycles** |
| **IL-3**<br>5.40 PM - 6.00 PM | **R. K. Singh**<br>Divisions of Toxicology1 and Endocrinology2, CSIR-Central Drug Research Institute, Jankipuram Extension, Lucknow-226 031, U.P., India<br>**Preclinical Toxicity Assessment of RISUGadv as A New Molecule** |
| **IL-4**<br>6.00 PM - 6.20 PM | **M. V. Raghavendra Rao**<br>Professor of Medical Microbiology, Immunology & Parasitology, Dean Students Affairs & Research Director, Avalon University School of Medicine, Sta. Rosaweg 122-124, Willemstad, Curaçao<br>**New thoughts in drug research to prevent teratogenicity** |
| **IL-5**<br>6.20 PM - 6.40 PM | **Ashoke Sharon**<br>Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India<br>**Carbocyclic nucleosides: A potential scaffold in Antiviral Drug Discovery** |

**Parallel Session – II B**

**Chairpersons: Dr. M. Sasidharan and Dr. Keshav Deo**

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| **PL-3**<br>4.30 PM - 5.00 PM | **Athina Athanasios Geronikaki**<br>Department of Pharmaceutical Chemistry, Aristotle University, Greece<br>**Design, synthesis and biological evaluation of new thiazole/thiadiazole derivatives** |
| **IL-6**<br>5.00 PM - 5.20 PM | **Thirumala Govender**<br>Discipline of Pharmaceutical Sciences, University of KwaZulu-Natal, Durban, South Africa<br>**Nano-antibiotics for Enhancing Treatment of Bacterial Infections** |
| **IL-7**<br>5.20 PM -5.40 PM | **Evans Coutinho**<br>Bombay College of Pharmacy, Kalina, Santacruz (E), Mumbai 400 098. India<br>**Tight Integration of Pharmacokinetics and Pharmacodynamics in the Design** |

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| | **of Leads - A Case Study** |
| **IL-8**<br>5.40 PM - 6.00 PM | **T. Narender**<br>Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow-226 031, UP., India<br>**Applications of NMR spectroscopy for Serendipitous Chemistry** |
| **IL-9**<br>6.00 PM - 6.20 PM | **Dipankar Koley**<br>Scientist, CSIR-Central Drug Research institute, Lucknow<br>**Acetal with Hydroxylactam: New Collaboration in Asymmetric Catalysis** |

**Poster Session –I**

**Chairpersons: Dr. Dipanker Koley**

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| 6.30 PM – 7.30 PM | **Poster Number 1 to 75** |
| 7.30 PM – 8.30 PM | **Cultural Programme** |
| **8.30 PM** | **Dinner** |

**Thursday, February 9, 2017**

**Parallel Session – III A**

**Chairpersons: Prof. Athina Athanasios Geronikaki and Dr. K.S. Lakshmi**

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| **PL-4**<br>9.00 AM - 9.30 AM | **Erik V. Van der Eycken**<br>Department of Chemistry, University of Leuven (KU Leuven), Laboratory for Organic & Microwave-Assisted Chemistry (LOMAC), Celestijnenlaan200F, Leuven, B-3001, Belgium<br>**Gold Nanoparticles Catalyzing Spirocyclizations under Microflow Conditions** |
| **PL-5**<br>9.30 AM - 10.00 AM | **Shirley W. I. Siu**<br>Department of Computer and Information Science, University of Macau, China<br>**Faster and Better Molecular Docking for Structure-based Drug Design with Swarm Intelligence Algorithms** |
| **IL-10**<br>10.00 AM - 10.20 AM | **Virinder S Parmar**<br>Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi, India<br>**Natural products-inspired discovery and development of anti-microbial, anti-inflammatory and antiplatelet agents** |
| **IL -11**<br>10.20 AM - 10.40 AM | **V. Gopal**<br>Professor, Head of the Department of Pharmacognosy and Principal, College of Pharmacy, Mother Theresa Post Graduate and Research Institute of Health Sciences, Puducherry, India<br>**Current Challenges in affordable and sustainable drug discovery from traditional Indian medicine** |
| **IL -12**<br>10.40 AM - 11.00 AM | **Ashok K Prasad**<br>Professor, Department of Chemistry, University of Delhi, Delhi, India<br>**Sugar-modified Nucleosides and Sugar-based Amphiphiles as Nanocarriers** |

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| **IL -13**<br>11.00 AM -11.20 AM | **Akhilesh Kumar Verma**<br>Department of Chemistry, University of Delhi, Delhi-110007, India<br>**Base-Mediated and Protection Free [4+2] Cycloadditions of Alkynes with Azadienes: An Efficient Assembly of Functionalized Quinolines** |
| **11.20 AM - 11.40 PM** | **Tea** |

**Parallel Session – III B**

**Chairpersons: Prof. Anamik Shah and Dr. P.M.S.Chauhan**

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| **PL-6**<br>9.00 AM - 9.30 AM | **Jyoti Chattopadhyaya**<br>Professor & Chair, Program of Chemical Biology, Dept. of Cell & Molecular Biology, Uppsala University, Sweden<br>**How genetic information is stored from RNA to DNA? Mechanism and BioMed Application** |
| **IL-14**<br>9.30 AM -9.50 AM | **Satpal Singh Badsara**<br>Assistant Professor & DST INSPIRE Faculty, MFOS Laboratory, Department of Chemistry, University of Rajasthan, Jaipur, Rajasthan, India<br>**Synthesis of Thio/Seleno Ethers and Esters Under Metal Free Conditions *via* C-H Functionalization** |
| **IL-15**<br>9.50 AM - 10.10 AM | **Diwan S Rawat**<br>Coordinator, M. Tech (Chemical Synthesis and Process Technologies), Department of Chemistry, University of Delhi, Delhi, India<br>**Molecular hybrid based drug design: A lesson from the nature** |
| **IL -16**<br>10.10 AM - 10.30 AM | **D. Sriram**<br>Department of Pharmacy, Birla Institute of Technology & Science-Pilani, Hyderabad campus, Jawahar Nagar, Hyderabad-500078, India<br>**Drug discovery strategies for the latent tuberculosis infection** |
| **IL -17**<br>10.30 AM - 10.50 AM | **Abhay Kotecha**<br>Division of Structural Biology, University of Oxford, UK<br>**Hybrid methods guide structure based vaccine design for picornaviruses** |
| **IL -18**<br>10.50 AM -11.10 AM | **Rakesh Shukla**<br>EX Chief Scientist & Head, Division of Pharmacology, CSIR-Central Drug Research Institute, Lucknow, 226031, India<br>**Intranasal Insulin: A Promising Treatment for Alzheimer Disease** |
| **11.20 AM - 11.40 PM** | **Tea** |

**Parallel Session - IV A**

**Chairpersons: Dr. N. Selvamurugan and Dr Rakeshwar Bandichor**

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| **IL-19**<br>11.40 AM - 12.00 PM | **Makarand Waikar**<br>ACS International India Pvt Ltd, 501-3, Jeevan Heights, Thorat Colony, Erandwane, Pune–411004, India<br>**Identifying novel substances by creative use of value added databases** |

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| **IL-20**<br>12.00 PM - 12.20 PM | **Anil Kumar**<br>Department of Chemistry, Birla Institute of Technology and Science, Pilani, India<br>**Synthesis of Bioactive Heterocyclic Compounds*via*Carbon-Hydrogen and Nitrogen-Hydrogen Bond Activation** |
| **IL-21**<br>12.20 PM - 12.40 PM | **O. P. Sidhu**<br>CSIR-National Botanical Research Institute, Rana Pratap Marg, Lucknow-226 001, India<br>**Metabolic variability among different accessions of guggul (Commiphora wightii) using GC-MS, HPLC and NMR spectroscopy** |
| **IL-22**<br>12.40 PM - 1.00 PM | **Ramesh Babu Boga**<br>BogaR Laboratories LLC, PO Box 1554, Suwanee, GA 30024, USA<br>**Nitric Oxide Synthase (NOS) Inhibitors: Past, Present, and the Future** |
| **1.00 PM - 2.20 PM** | **Lunch** |

**Parallel Session - IV B**

**Chairpersons: Dr. K. Ilango**

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| **IL-23**<br>11.40 AM - 12.00 PM | **Vinay Tripathi**<br>Chief Scientist & Head S&T Management Unit, CSIR-Central Drug Research Institute, Lucknow, India<br>**Intellectual Property Rights; An Overview** |
| **IL-24**<br>12.00 PM - 12.20 PM | **A. JesuArockia Raj**<br>Division of Fisheries Biotechnology & Molecular Biology, Department of Biotechnology, Faculty of Science and Humanities, SRM University, Kattankulathur 603 203, Chennai, India<br>**Aquatic antimicrobial peptides (AMPs): Natural templates for design new antimicrobial compounds** |
| **IL-25**<br>12.20 PM - 12.40 PM | **Devdutt Chaturvedi**<br>Department of Chemistry, School of Physical & Material Sciences, Mahatma Gandhi Central University, Motihari-845401(East Champaran), Bihar, India<br>**Greener syntheses employing carbon dioxide: An easy access for the syntheses of biologically potent scaffolds** |
| **IL-26**<br>12.40 PM - 1.00PM | **Gautam Panda**<br>Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Sector 10, Sitapur Road, Jankipuram Extension, Lucknow-226031, UP, India<br>**Amino Acids Chirons: Quest for Bioactive Alkaloids and Steroidomimetics** |
| **1.00 PM - 2.20 PM** | **Lunch** |

**Parallel Session - V A**

**Chairpersons: Dr. M. S. Umashankar and Dr. V.Chitra**

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| **PL-7**<br>2.20 PM - 2.50 PM | **Wafaa M. Abdou**<br>Chemical Industries Division, National Research Centre, Elbohouth St., Dokki, |

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| | Cairo, Egypt<br>**Current Benefits of bisphosphonates in oncology** |
| **O-1**<br>2.50 PM - 3.00 PM | **Ranjan Khunt**<br>Chemical Research Laboratory, Department of Chemistry, Saurashtra University, Rajkot-360005 (Gujarat) India<br>**Ugi Multicomponent Reaction and Insilico Study of Fluorinated carboxamides derivatives as an anti-tubercular agents** |
| **O-2**<br>3.00 PM - 3.10 PM | **John J. Georrge**<br>Department of Bioinformatics, Christ College, Rajkot-360005, India<br>**Identification of Novel Drug Targets through subtractive genomics approach** |
| **O-3**<br>3.10 PM -3.20 PM | **Rashmi Gaur**<br>Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow<br>**Natural product and its derived compounds as a source of new lead in drug discovery** |
| **O-4**<br>3.20 PM - 3.30 PM | **Manorama Singh**<br>Assistant Professor, Department of Chemistry, Guru Ghasidas Vishwavidyalaya (a Central University), Bilaspur – 495 009, C. G., India<br>**Fe-SPINEL DOPED Naf/DMAP-GO: NANOCOMPOSITE FOR MOLECULAR RECOGNITION** |
| **O-5**<br>3.30 PM - 3.40 PM | **Subhash Chander**<br>Medicinal Chemistry Research Laboratory, Department of Pharmacy, Birla Institute of Technology & Science, Pilani-333031. Rajasthan, India<br>**Design, synthesis and anti-tubercular activity of novel tetrahydroquinoline based hydrazides** |
| **O-6**<br>3.40 PM - 3.50PM | **Jennifer Fernandes**<br>Dept. of Pharmaceutical Chemistry, NGSM Institute of Pharmaceutical Sciences, Nitte University Deralakatte, Mangalore, India<br>**PROTECTIVE POTENTIAL OF *AVERRHOA BILIMBI* LEAF EXTRACT ON ALCOHOL AND ACETAMINOPHEN INDUCED HEPATOTOXICITY** |
| **O-7**<br>3.50 PM - 4.00 PM | **Mohd. Athar**<br>CCG@CUG, School of Chemical Sciences, Central University of Gujarat, Sector 30, Gandhinagar-382030, India<br>**Density Functional Theory based Investigation of Structure and Conformational Equilibrium Of Oxacalix[4]arene** |
| **4.00 PM - 4.20 PM** | **Tea** |

**Parallel Session - V B**

**Chairpersons: Prof. Mahesh K. Lakshman and Dr. S. Sangeetha**

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| **IL-27**<br>2.20 PM - 2.40 PM | **Nisheeth C Desai**<br>Department of Chemistry, DST-FIST, Sponsored Department, Mahatma Gandhi campus, Maharaja KrishnakumarsinhjiBhavngar University, Bhavnagar - 364 002, India |

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| | **Landscaping of biological active of novel hybrid heterocyclic as antimicrobial, antitubercular and anticancer agents – A journey of one decade** |
| **IL-28**<br>2.40 PM - 3.00 PM | **Sunil K. Sharma**<br>Department of Chemistry, University of Delhi, Delhi 110 007, India<br>**Synthesis and Kinase Inhibition Study of Pyridylpyrimidinylaminophenyl Derivatives** |
| **O-8**<br>3.00 PM - 3.10 PM | **Soni Shaikh**<br>1Advanced Center forChronicDisease (ACCDiS) & Center for Molecular Studies of theCell (CEMC), Facultad de Ciencias Químicas y Farmacéuticas & Facultad de Medicina, Universidad de Chile, Santiago, Chile<br>**Stim1 inhibitor ML9 promotesdeath signals in cultured ratcardiomyocytes** |
| **O-9**<br>3.10 PM - 3.20 PM | **Selvaraj Jubie**<br>Department of Pharmaceutical Chemistry, Jagadguru Sri Shivarathreeshwara University, Mysore, India<br>**A Novel Sulpha Lipid as Human Topoisomerase I & II inhibitor: Isolation and its Cytotoxicity Screening** |
| **O-10**<br>3.20 PM - 3.30 PM | **Vijai K. Rai**<br>Assistant Professor, Department of Chemistry, Guru Ghasidas Vishwavidyalaya (a Central University), Bilaspur – 495 009, C. G., India<br>**β-LACTAM RING: SYNTHESIS AND ROLE IN DRUG DISCOVERY** |
| **O-11**<br>3.30 PM -3.40 PM | **Prabodh Ranjan**<br>School of Chemical Sciences, Central University of Gujarat, Sector-30, Gandhinagar-382030, Gujarat, India<br>**Exploration of Interaction Zones of β-tubulin Colchicine Binding Domainof Helminths and Binding Mechanism of Anthelmintics** |
| **O-12**<br>3.40 PM -3.50 PM | **S.Umamaheswari**<br>Professor, Department of Pharmacology, Faculty of Pharmacy, Sri Ramachandra University, Chennai, India<br>***INVITRO* HYPOGLYCEMIC POTENTIAL OF SELECTED DIHYDROXY FLAVONES** |
| **O-13**<br>3.50 PM - 4.00 PM | **P. A. Abhinand**<br>Department of Bioinformatics, Sri Ramachandra University, Porur, Chennai – 600 116, India<br>**Artificial Neural Network Model to Recognize Potential MAO-B inhibitors for Parkinson's Treatment** |
| **4.00 PM - 4.20 PM** | **Tea** |

**Parallel Session - VI A**

**Chairpersons: Dr. P. R. Kumar**

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| **O-14**<br>4.20 PM - 4.30 PM | **Sai Prathima Parvathaneni**<br>Catalysis Laboratory, Inorganic and Physical Chemistry Division, CSIR-Indian Institute of Chemical Technology (IICT),Tarnaka, Hyderabad –500 607, India<br>**Regioselective *ortho*-Halogenation of Aryl C-H bonds** |

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| **O-15**<br>4.30 PM - 4.40 PM | **R. Elancheran**<br>Drug Discovery Laboratory, Life Sciences Division, Institute of Advanced Study in Science and Technology, Guwahati-781035, India<br>**Design and development of flavonoid derivatives as androgen receptor antagonists** |
| **O-16**<br>4.40 PM - 4.50 PM | **Zahid Yaseen**<br>Department of Chemistry, Islamic University of Science and Technology, Kashmir 192122, India<br>**Design and development of flavonoid derivatives as androgen receptor antagonists** |
| **O-17**<br>4.50 PM - 5.00 PM | **Venkatesh Kumaresan**<br>Division of Fisheries Biotechnology & Molecular Biology, Department of Biotechnology, Faculty of Science and Humanities, SRM University, Kattankulathur, Chennai, Tamil Nadu 603 203, India<br>**Discovery of antimicrobial peptides from proteome dataset using a novel *insilico*Cluster approach** |
| **O-18**<br>5.00 PM - 5.10 PM | **Ritu Kapoorr**<br>Division of Fisheries Biotechnology & Molecular Biology, Department of Biotechnology, Faculty of Science and Humanities, SRM University, Kattankulathur, Chennai, Tamil Nadu 603 203, India<br>**Silver-Catalyzed Denitrative Sulfonylation of Nitrostyrenes: A Convenient Approach to (*E*)-Vinyl Sulfones** |
| **O-19**<br>5.10 PM - 5.20 PM | **Mahesh. S. Krishna**<br>Diabetes Biology Lab, Division of Cardiovascular and Diabetes Biology, Rajiv Gandhi Centre for Biotechnology, Poojappura, Thiruvananthapuram, Kerala, India<br>**Modulation of Glut4 during adipogenesis in 3T3L1 correlates with expression of LXR alpha** |
| **O-20**<br>5.20 PM - 5.30 PM | **Priya Rani M**<br>Department of Chemistry, University of Kerala, Kariavattom campus, Thiruvananthapuram 695 581, Kerala, India<br>**Various Spectral Methods for the Characterization of Alpha-amylase Inhibitors from the Roots of *Stereospermum colais*** |
| **O-21**<br>5.30 PM - 5.40 PM | **Hardik Bhatt**<br>Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad 382 481. India<br>**Design and Synthesis of Hit Molecules Bearing Novel Pteridine Scaffold as Dual Aurora-B and CDK2 Kinase Inhibitors as Apoptosis Inducer** |
| **O-22**<br>5.40 PM - 5.50 PM | **Pankaj Dwivedi**<br>Department of Precision Machinery and Precision Instrumentation, University of Science and Technology of China, Hefei, Anhui, 230027, People's Republic of China<br>**Coaxial electrospray fabrication of paclitaxel loaded solid lipid microparticles for cancer targeting** |
| **O-23**<br>5.50 PM - 6.00 PM | **Mohsin Y. Lone**<br>School of Chemical Sciences, Central University of Gujarat, Gandhinagar-382030, Gujarat, India |

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| | **The Discovery of Novel Enoyl-acyl Carrier Protein Reductase Inhibitors: A Multiple Complex Based Pharmacophore Modelling Approach** |

**Parallel Session - VI B**

**Chairpersons: Dr. Sudhir Singh and Dr. N. Damodharan**

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| **PL-8**<br>4.20 PM - 4.50 PM | **Eng. Karol Grela**<br>Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Poland<br>**Catalytic Olefin Metathesis at the Dawn of Implementation in Green Pharmaceutical Production** |
| **O-24**<br>4.50 PM - 5.00PM | **D. N. Singh**<br>Department of Chemistry, K.S. Saket PG College, Dr. RML Avadh University, Faizabad- 224001, India<br>**Isolation, characterization and biological activity of a new ursane-triterpene from *Phlebophyllum kunthianum*** |
| **O-25**<br>5.00 PM - 5.10 PM | **Jignasu P Mehta**<br>Analytical Chemistry Division, Department of Chemistry, (UGC NON-SAP & DST-FIST sponsored Department), Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar, India<br>**Antimicrobial and antioxidant activities of minor millet extracts** |
| **O-26**<br>5.10 PM - 5.20 PM | **Keshri Nath Tiwari and Rinku Choubey**<br>Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), ITI Compound, Raebareli 229 010, India<br>**An efficient and direct synthesis of substituted 2-phenylquinoline-4-carboxamides from 3-substituted-3-hydroxyindolin-2-ones** |
| **O-27**<br>5.20 PM - 5.30 PM | **Sabir Hussain**<br>Department of Chemistry, Aggarwal College, Ballabgarh (M.D University Rohtak), Haryana 121006, India<br>**One-pot conversion of Ofloxacin using tetra butyl ammonium bromide and their Biological Activity** |
| **O-28**<br>5.30 PM - 5.40 PM | **Anil Kumar**<br>Department of Biotechnology, SMVD University, Katra, J&K, 182320, India<br>**Syntheses of Families of Enantiopure and Diastereopure Octahedral Cobalt Catalysts and their utility in Organic Synthesis** |
| **O-29**<br>5.40 PM - 5.50 PM | **Priyanka Saha**<br>Department of Zoology, St. Xavier's College, Ranchi- 834001, Jharkhnad, India<br>**GENOMIC ANALYSIS OF TOLERANT BACTERIA OBTAINED FROM *PARTHENIUM HYSTEROPHORUS* L. AMENDED SOIL** |
| **O-30**<br>5.50 PM - 6.00 PM | **K. Sesha Maheswaramma**<br>Assistant Professor in Chemistry, Jawaharlal Nehru Technological University Anantapur College of Engineering Pulivendula, Andhra Pradesh-516390, India<br>**Remarkable anticancer activity of ternary copper (II) and oxovanadium(IV) complexes in red light with low dark toxicity** |
| **O-31** | **T. Anjali**<br>Department of Chemistry, JNTUACEP, Pulivendula, Kadapa(Dt), Andhra Pradesh- |

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| 6.00 PM - 6.10 PM | 516390, India<br>**Review of chemical approaches on drug development and sustainability (Alchemy to till)** |

**Poster Session – II**

**Chairpersons: Dr. C. Gopalakrishnan and Dr. R. Ramajayam**

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| 6.10 PM – 7.30 PM | **Poster Number 75 onwards** |
| 7.30 PM – 8.30 PM | **Cultural Programme** |
| **8.30 PM** | **Dinner** |

**Friday, February 10, 2017**

**Session – VII**

**Chairpersons: Prof. Wafaa M. Abdou**

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| **PL-9**<br>9.30 AM - 10.00 AM | **Victor Kartsev**<br>Full member of RANS, Honorary Academician of Russian Academy of Arts, VP, CSO&CEO InterBioScreen, Russia<br>**Abstract Awaited** |
| **PL-10**<br>10.00 AM -10.30 AM | **Johan Van der Eycken**<br>Laboratory for Organic and Bioorganic Synthesis, Ghent University, Department for Organic and Macromolecular Chemistry, Krijgslaan 281 (S.4), B-9000 GHENT, Belgium<br>**TOTAL SYNTHESIS AND BIOLOGICAL EVALUATION OF PELOFEN, A SIMPLIFIED ANALOGUE OF PELORUSIDE A WITH MICROTUBULE-STABILIZING ACTIVITY** |
| **PL-11**<br>10.30 AM - 11.00 AM | **Anil Kumar Singh**<br>IIT Mumbai, Former Vice Chancellor, University of Allahabad, India<br>**Molecular Caging – a novel strategy for light-mediated targeted release of bioactive compounds** |
| **IL-29**<br>11.00 AM - 11.20 AM | **Rakesh Rawal**<br>Senior Scientific Officer & Head, Div. of Medicinal chemistry & Pharmacogenomics, Dept. of Cancer Biology, The Gujarat Cancer & Research Institute, Ahmedabad, Gujarat, India<br>**A paradigm shift in natural product based drug discovery from classical to empirical approach** |
| **IL-30**<br>11.20 AM - 11.40 AM | **Ajay K. Sah**<br>Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, India<br>**Synthesis of N-glyconjugates and their applications in biological sciences** |
| **O-32**<br>11.40 AM -11.50 AM | **Rambabu Dandela**<br>Dept. of Chemistry and the National Institute for Biotechnology in the Negev, Ben-Gurion University of the Negev, Be'er Sheva, Israel<br>**Synthesis and evaluation of a tag-free photoactive phospho-ceramide analogue-1** |

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| | **(PCERA-1) probe to study immunomodulation in macrophages** |
| **O-33**<br>11.50 AM -12.00 | **Suraj K. Singh**<br>Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi, India<br>**Chemoenzymatic synthesis, nanotisation and anti-*Aspergillus* potential of novel fluconazole analogues** |
| **O-34**<br>12.00 -12.10 PM | **H. M. Patel**<br>Sardar Patel University, Department of Chemistry, University Campus, Vallabh Vidyanagr- 388 120, Gujarat, India<br>**Green Approach for Synthesis of Bioactive Hantzsch 1,4-Dihydropyridine Derivatives Based on Thiophene Moiety via Multicomponent Reaction** |
| **O-35**<br>12.10 PM -12.20 PM | **Pankaj Kumar Singh**<br>Chemical Research Division, Sunpharmaceutical Industries Ltd, Gurgaon, Haryana, 122004, India<br>**Micellar catalysis a greener approach in pharmaceutical industry** |
| **O-36**<br>12.20 PM -12.30 PM | **S. Vijayaraj**<br>Department of Pharamceutical Analysis,Sree Vidyanikethan College of Pharmacy, Tirupathi, AP, India<br>**PHARMACOKINETIC STUDY OF AMINO ACID PRODRUG OF GLICLAZIDE BY LC-MS/MS METHOD IN RABBIT PLASMA** |
| **O-37**<br>12.30 PM -12.40 PM | **Pinku Kaswan**<br>Department of Chemistry, Birla Institute of Technology & Science, Pilani 333 031, India<br>**Synthesis of 3-Aroylimidazo[1,2-*a*]pyridine, and Functionalization of Imidazo[1,2-*a*]pyridines using Vanadium Catalyst** |
| **O-38**<br>12.40 PM -12.50 PM | **A. Kalpana**<br>Department of Chemistry, JNTUACEP, Pulivendula, Kadapa(Dt), A.P-516390, India<br>**Advanced Approaches of Green Principles to AchieveSustainability of Modern Domestic life** |
| **O-39**<br>12.50 PM -1.00 PM | **Faraz Shaikh**<br>The Gujarat Cancer & Research Institute, Ahmedabad, Gujarat, India<br>**Design, Synthesis in silico high throughput screened and discovery of novel human p-glycoprotein inhibitors as MDR cancer** |
| **O-40**<br>1.00 PM -1.10 PM | **Sunil Singh**<br>Research Scholar, Department of Pharmacy, Mewar University, Gangrar, Chittorgarh, Rajasthan, India<br>**First Total Synthesis and Biological Potential of a Heptacyclopeptide of Plant Origin** |
| **O-41**<br>1.10 PM -1.20 PM | **Vijaya Laxmi. S**<br>K L University, Guntur, Andhra Pradesh, India<br>**Triflic anhydride mediated room temperature Synthesis of 3-substituted Benzofurans** |
| **O-42**<br>1.20 PM -1.30 PM | **Jignesh H. Trivedi**<br>P. G. Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India |

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| | **Synthesis and Characterizationof Sodium Salt of Carboxymethylated Sodium Alginate graftedPoly (methyl acrylate)** |
| 1.30 PM - 2.15 PM | **Valedictory Session** |
| 2.15 PM - 3.00 PM | **Lunch** |
| 3:00 PM – 4:30 PM | **ISCB General Body** |

# PLENARY

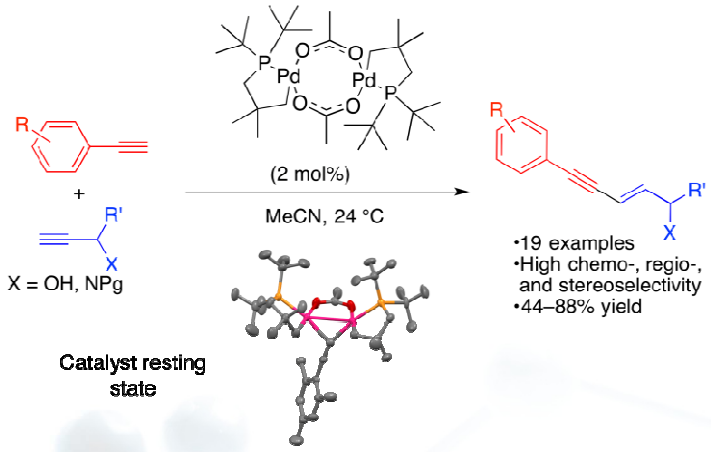
PL-1

# UNRAVELING THE IMPACT OF LIGAND STERIC ELECTRONIC PROPERTIES ON METAL-CATALYZED BOND-FORMING REACTIONS

**Kevin H. Shaughnessy***

*Department of Chemistry, The University of Alabama, Tuscaloosa, AL 35487, USA*
*E-mail: kshaughn@ua.edu*

Homogeneous metal-catalyzed reactions, such as cross-coupling, olefin metathesis, and carbonylation reactions, play critical roles in the synthesis of biologically active molecules and pharmaceuticals. These powerful reactions have long played key roles in the drug discovery process and are increasingly being employed in process level syntheses. The development of high activity catalysts requires an understanding of the mechanism of these processes and the role that ligands play in modifying the reactivity of metal centers. Our group has a long-standing interest in developing an understanding of the role of steric and electronic properties of ligands in catalyst performance. Phosphine ligands with conformationally flexible substituents, such as neopentyl or benzyl, have proven to afford catalysts with interesting synthetic applications.[1-3] The highly flexible trineopentylphosphine ligand affords catalysts that are highly active for the C–C and C–N coupling of sterically demanding substrates.[4] In contrast to sterically rigid ligands, such as tri-*tert*-butylphosphine, trineopentylphosphine provides a highly active catalyst for coupling of sterically demanding aryl halides and aryl amines. The neopentylphosphine family of ligands provides for fine control of the product selectivity of Heck couplings of cyclic alkenes to afford either the kinetically or thermodynamically preferred olefin product.[5] Neopentylphosphines readily form metallacyclic complexes by C–H activation of the neopentyl substituent. The [Pd(μ-$\kappa^2$-*O*,*O*-OAc)( $\kappa^2$-*C*,*P*-(*t*-Bu)$_2$PCH$_2$C(Me)$_2$CH$_2$)]$_2$ complex selectively affords *E*-5-aryl-2-en-4-yn-1-ol products in good yields under mild conditions with high chemo-, regio-, and stereoselectivity.[6]

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**PL-2**

# A Novel Approach to C6 Benzotriazolyl Purine Nucleoside Analogues

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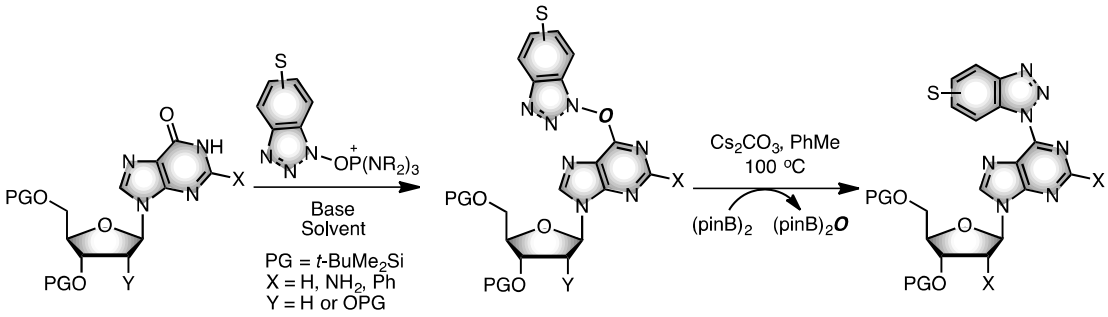
We have previously described deoxygenation reactions of amine *N*-oxides to amines with bis(pinacolato)diboron [(pinB)$_2$] and bis(catecholato)diboron [(catB)$_2$].[1] Subsequently, we showed the conversion of 1-hydroxy-1*H*-benzotriazoles to 1*H*-benzotriazoles with $B_2(OH)_4$, which also involves a N–O bond deoxygenation.[2] Building on these experiences we have studied a novel approach to C6 benzotriazolyl purine nucleoside analogues.[3] Briefly, reactions of amide linkages in inosine, 2'-deoxyinosine, guanosine, and 2'-deoxyguanosine with phosphorus-based peptide-coupling agents, such as (benzotriazol-1-yloxy)trisdimethylamino-phosphoniumhexafluorophosphate (BOP), give facile access to $O^6$-(benzotriazol-1-yl) purine nucleosides. These are exceptionally useful convertible nucleoside analogues, as we have previously demonstrated.[4–6] However, upon exposure to (pinB)$_2$, these compounds undergo a C–O–Ndeoxygenation and C–N bond formation, leading to C6 benzotriazolyl purine nucleoside analogues. No metal is needed for this novel transformation. Details and mechanistic studies will be described.




**Acknowledgments**

Support of this work by NSF Grant CHE-1265687 and a PSC CUNY award to MKLis gratefully acknowledged. Infrastructural support at CCNY was provided by NIH grant G12MD007603 from the National Institute on Minority Health and Health Disparities.

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**PL-3**

## Design, synthesis and biological evaluation of new thiazole/thiadiazole derivatives

**Geronikaki**[1], M. Fesatidou[1], E. Tsolaki[1], E. Pitta[1], A. Ciric[2], J.Glamočlija[2], M.Sokovic[2]

[1]*Department of Medicinal Chemistry, School of Pharmacy, Aristotle University of Thessaloniki, Greece.*
[2]*Mycological Laboratory, Department of Plant Physiology, Institute for Biological Research, Siniša Stanković, University of Belgrade, Bulevar Despota Stefana 142, 11000, Belgrade, Serbia.*
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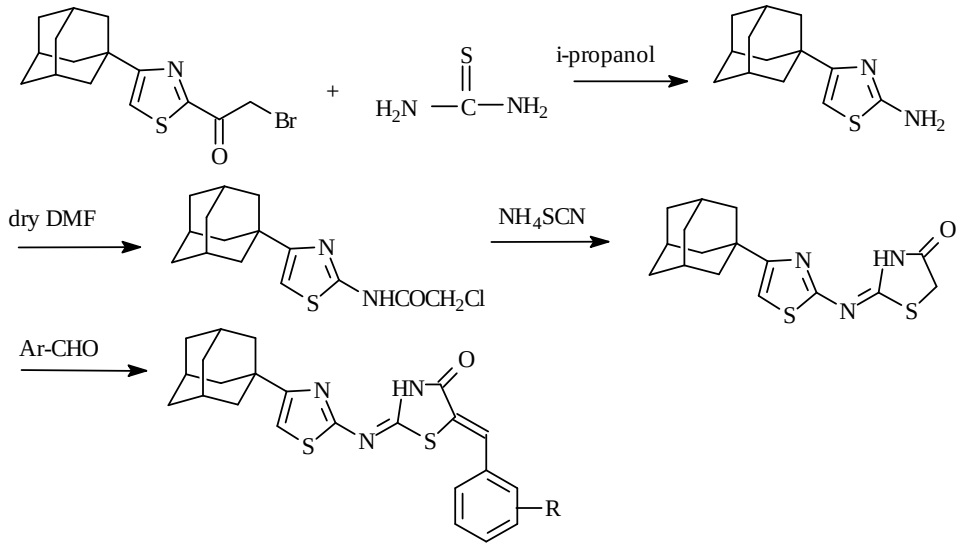
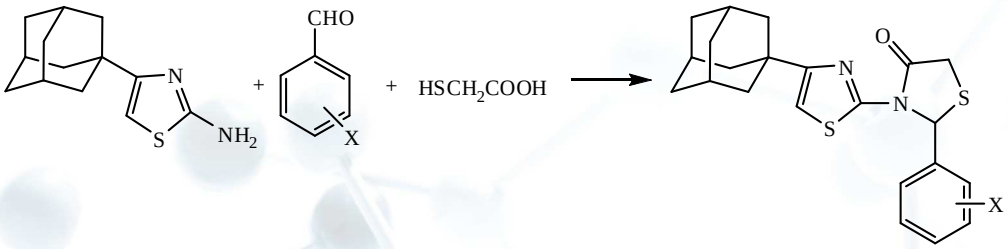
Despite the success to date in development of antimicrobial agents, the inexorable, ongoing emergence of resistance worldwide continues to spur the search for novel compounds to replace or supplement conventional antibiotics and antifungals. Taking into account the interesting antimicrobial and chemical properties of thiazole, thiadiazole as well as adamantane derivatives, herein is presented the synthesis and evaluation of antimicrobial activity of twenty compounds presented in Schemes 1 and 2.




Scheme 1.




Scheme 2.

The antimicrobial assay was carried out by microdilution method. For the evaluation of the antifungal activity of the compounds, the following fungi were used: *A. ochraceus*,, *A. fumigatus*, *A. niger*, *A. versicolor*, *A. flavus*, *P. funiculosum*, *P. ochrochloron*, *T. viride*, *C. albicans* and *F. Sporotrichoides* while for the antibacterial tests were used Gram-negative bacteria *E. coli*, *P. aeruginosa*, *S. typhimurium*, *En. faecalis* and Gram-positive bacteria *L. monocytogenes*, *B. cereus*, *M. flavus*, *En.*

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

The tested compounds exhibited outstanding antimicrobial activity, being in most of the cases more potent than reference drugs.
The synthesized compounds having thiazolidine-4-one moiety have been docked at the active side of the *Staphylococcus aureus* Mur B active site (PDB: 1HSK). The most active compound in the series was found to have hydrogen bond contact with the backbone nitrogen of GLY249. The thiazolidine-4-one is mainly responsible for the activity of the molecule as it is a potential surrogate of the di-phosphate moiety present in UDP-N-acetylenolpyruvylglucosamine.[1]

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**PL-4**

## Gold Nanoparticles Catalyzing Spirocyclizations under Microflow Conditions

**Erik V. Van der Eycken**

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Gold catalysis utilizing supported gold nanoparticles is an emerging topic in the intensively studied domain of gold-catalyzed reactions. Supported gold nanoparticles combine the advantageous features of homo- and heterogeneous catalysis by merging the selective activation of π-systems with an uncomplicated recycling of the catalyst. Therefore, they provide opportunities to facilitate the application of gold catalysis on a larger scale. Nonetheless, in order to allow an application on an industrial scale, gold-catalyzed processes must be improved with regard to cost, productivity, robustness and environmental sustainability. A logical solution to overcome such issues is the use of a continuous-flow process utilizing highly active supported gold nanoparticles in a packed-bed reactor. The combination of heterogeneous gold catalysis with microreactor technology offers various advantagescompared to batch processes. Besides apparentbenefits such as enhanced mixing, improved heattransfer, and safer reaction conditions, the use ofa packed-bed reactor can increase selectivity and facilitatechallenging transformations. Under continuous-flow conditions, usually short residence timesare observed due to the increased amount of catalyst/reactant in the packed bed, resulting in less degradationof sensitive substrates. Moreover, the use of a catalyst bed facilitates catalystrecycling and reuse, thereby reducing the amountof metal impurities in the final product.Recently, our international group developed a novel heterogeneous gold catalyst, consisting of gold nanoparticles onan Al-SBA15 support, for post-Ugicycloisomerizations. The reaction enabled rapid and efficient access to variousspiroindolines. In terms of reactivity, selectivity and productivity, the reportedprotocol proves to be superior to previous reports. The main reason for thesuperiority is the very high catalyst to substrate ratioin the packed-bed reactor.Moreover no detectable leaching of the Au@Al-SBA15 catalytic bed was noted.

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PL-5

## Faster and Better Molecular Docking for Structure-based Drug Design with Swarm Intelligence Algorithms

**Shirley Weng In Siu**

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*E-mail: shirleysiu@umac.mo; Web: http://cbbio.cis.umac.mo*

Protein–ligand docking has become an important step in modern structure-baseddrug design. Given a biological target related to the disease of interest, the dockingprogram helps to decide if a small molecule ligand can bind to the target proteinwith a desirable level of affinity. Essentially, the flexible ligand docking can be seen as an optimization problem that aims to identify the lowest energy ligand binding pose out of all possible ligand's positions, orientations, and torsional angles in relative to the protein. Various optimization algorithms such as Monte Carlo (MC) and Genetic algorithm (GA) have been widely used. However, the main disadvantage of these methods is slow convergence, which leads to inefficiency and low accuracy. This talk will discuss the recent set of optimization algorithms, namely Particle Swarm Optimization (PSO) and Cuckoo Search (CS) which are based on the food-looking or breeding behavior of swarms. Results showed that our docking method based on swarm global search and modified Fletcher–Goldfarb–Shannon (BFGS) local search can achieve both speed and accuracy improvements over MC algorithm implemented in Autodock Vina. When comparing to other PSO docking programs and state-of-the-arts docking methods such as Glide, Surflex and AutoDock, our method achieves the highest success rate using the GOLD benchmark dataset.

**PL-6**

## How genetic information is stored from RNA to DNA? Mechanism and BioMed Application

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*Professor \& Chair, Program of Chemical Biology, Dept. of Cell & Molecular, Biology, Uppsala University, Sweden*

Abstract Awaited

PL-7

# Current Benefits of bisphosphonates in oncology

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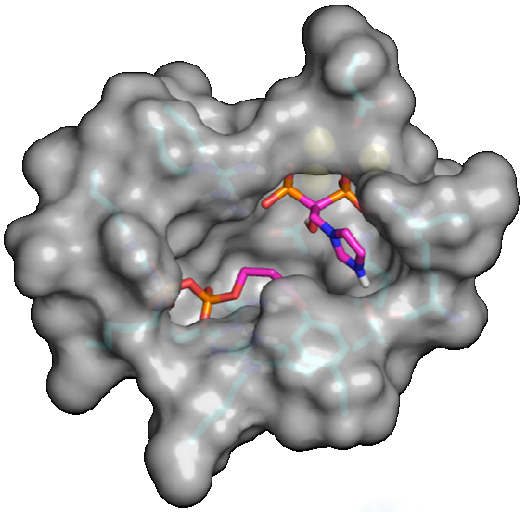
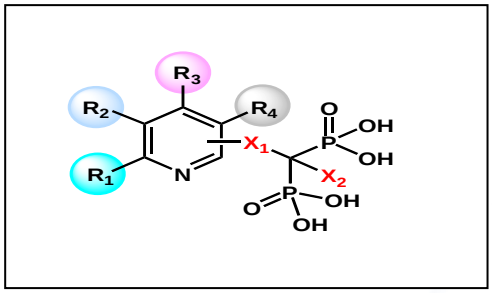
In addition to inhibiting bone resorption, and chronic arthritis, bisphosphonates (BPs) have also been shown to exhibit anti-tumor effects. *In vitro*, BPs inhibit proliferation and induce apoptosis in cultured human breast cancer cells. There is now a much greater appreciation of the benefits of introduction of BPs in oncology, which has dramatically changed the management of patients with metastatic bone disease. Recently, BPs have been, however, proven to be the drugs of choice to: i- Decrease in bone resorption in tumor bone disease. ii- Decrease in hypocalcemia as a result of diminution of bone resorption that leads to a big decrease of new osteolytic lesions, and iii- Decease of fractures, which results in amelioration of pain and an improvement of the quality of life [1]. This antitumor potency of BPs, particularly *N*-BPswas attributed to the differences of their molecular mechanism of action. Thus, BPs can be grouped in two main different classes: first-generation is non-*N*-BPs and the second generation is *N*-BPs. First-generation of BPs, such as clodronate and etidronate, are metabolized intracellular to analogues of ATP by inhibiting ATP-dependent enzymes. In contrast, second-*N*-BPs, generation such as pamidronate and zoledronate, interfere with mevalonate biosynthetic pathway, by inhibiting farnesyldiphosphate (FPP) synthase [2]. Our recent, and present work considered an elaboration of a novel seriesof nitrogen and/or sulfur containing BPs. Several of these *N*-BPs reflected remarkable antitumor activity against breast, ovarian, and prostatecarcinoma cell lines.






Mechanism of action of *N*-BPs

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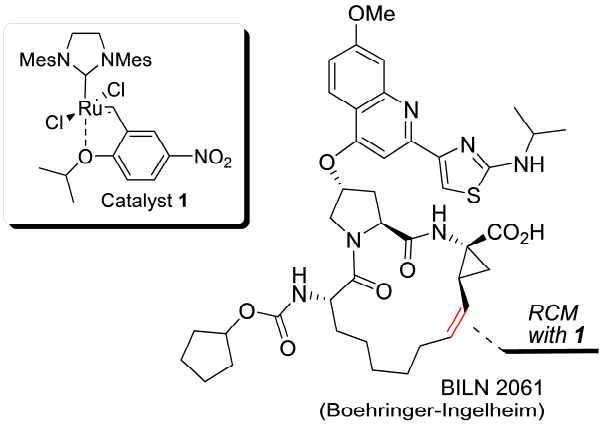
**PL-8**

# Catalytic Olefin Metathesis at the Dawn of Implementation in Green Pharmaceutical Production

**Prof. Dr. Eng. Karol Grela***

*Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Poland*

**Abstract:**




In the last decade of the 20th century, the catalytic olefin metathesis reaction has gained a real significance in advanced organic synthesis. The development of well-defined catalysts and the understanding of the reaction mechanism have revolutionized retro-synthetic planning in total synthesis and in medicinal chemistry worldwide [1]. The variety of metathesis catalysts now available on the market as well as the number of commercial players involved, are increasing. In addition new applications of metathesis are being constantly developed, including sustainable production of API molecules. We wish to present our contribution to the exciting field of metathesis by the discovery and development of very efficient EWG activated ruthenium olefin metathesis catalysts, and their applications in pharmaceutical industry [2].

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**PL-9**

## Targeted modification and virtual screening of Natural Products (Major InterBioScreen Ltd. Research Project)

**Victor Kartsev**

*Full member of RANS, Honorary Academician of Russian Academy of Arts, VP, CSO&CEO InterBioScreen*

Abstract Awaited

**PL-10**

# TOTAL SYNTHESIS AND BIOLOGICAL EVALUATION OF PELOFEN, A SIMPLIFIED ANALOGUE OF PELORUSIDE A WITH MICROTUBULE-STABILIZING ACTIVITY

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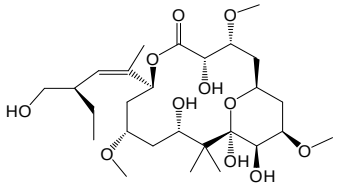
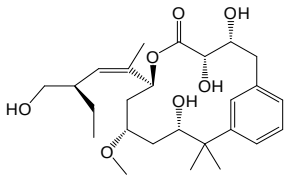
[b]*Laboratory for Experimental Cancer Research, Department of Radiation Oncology and Experimental Cancer Research, Ghent University, De Pintelaan 185 (P.7), B-9000 Ghent, Belgium*

Peloruside A (**1**) is a novel macrolide with potent anti-cancer activity, discovered in 2000 from a marine sponge [1]. Like Paclitaxel (**2**) and Epothilon (**3**), Peloruside A is a microtubule-stabilizing agent, but it binds to a different binding site [2] and shows a better activity against multidrug-resistant cancer cell lines. Moreover, the presence of several hydroxyl groups causes a better solubility in the blood stream. The binding site at □-tubuline and the biologically active conformation of (+)-Peloruside were confirmed in 2006 by Miller *et al*. [3a] via NMR and in 2014 by Steinmetz *et al.* [3b] via XR-analysis. The absolute configuration was established via total synthesis by De Brabander *et al*. [4]. Since then, a few total syntheses have been reported [5].

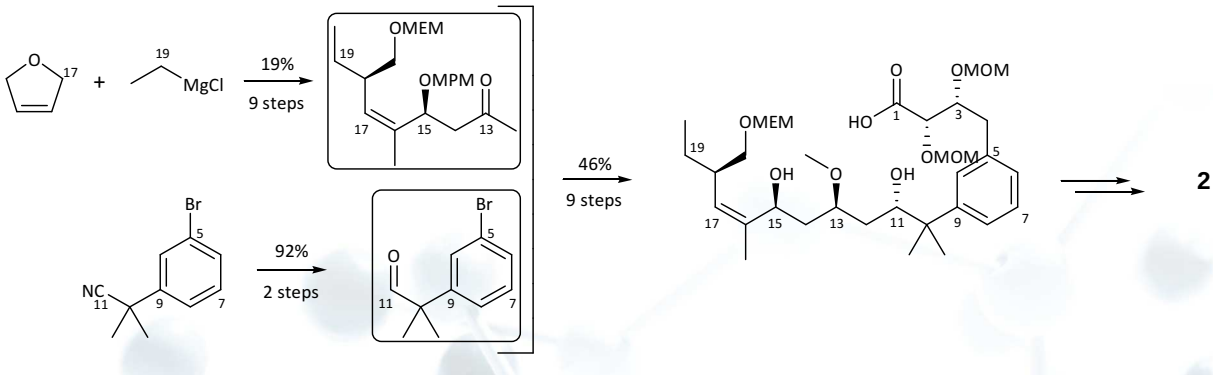


**1 Peloruside A**



**2 Pelofen**

In our endeavour for designing simplified analogues of Peloruside, we developed a modular synthesis (below) for Pelofen (**2**), possessing a simple phenyl ring instead of the pyranose ring. Biological screening revealed that this compound still shows pronounced microtubule stabilizing activity, thus rendering it highly promising as a potential lead for cancer treatment [6].

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**PL-11**

# Molecular Caging – a novel strategy for light-mediated targeted release of bioactive compounds

**Anil Kumar Singh**

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Molecular caging is a technique in which a bioactive molecule is rendered inactive by covalently linking it to a light-sensitive group. When required, the caged molecule can be liberated in its active form by irradiation of the cage. The photo-release of molecule in its active form can be achieved in site-, time- and concentration-controlled manner. This makes molecular caging a very powerful technique for achieving spatially and temporally controlled release of bioactive molecules with wide applications in biology, chemistry, medicine and physiology. Some of the applications of molecular caging include processes as diverse as light-controlled enzymatic catalysis, activity of neurotransmitters, pro-drug activation and targeted drug delivery, photo-control of pharmacological activity, building or isolating libraries in combinatorial chemistry, photolithography, light-directed synthesis of high-density molecular arrays, protein folding, photoactivation of gene expression, time-resolved x-ray crystallography, and photorelease of caged reagents in chemical transformations.[1-5]

Success of this strategy in biological and biomedical applications much depends upon the availability of photo-activators and switches suitable under physiological conditions. Several photosensitive groups including phenacyl–, *o*–hydroxycinnamoyl–, coumarin–, *o*-nitrobenzyl and napthyl, quinolines and many others have been examined for their efficacy as photo-trigger. Attention has also been paid towards development of fluorescent cages, which if used for un-caging orthogonally together with fluorescence microscopy, provide valuable information about cellular events and functions. In recent times, design of multi-photon sensitive probes has received much attention. This is primarily because of the availability of mode-locked, Ti:sapphire lasers and improvement in spatial resolution for controlled release. Currently, development of new chromophores with excellent two-photon cross-sections and applicability under physiological conditions is one frontier for caging probe development. Another frontier for new developments in caging technology is the design of photoreversible caged compounds. This presentation, while focusing on our efforts towards design, properties and applications of molecular cages, will also review recent accomplishments in the field and highlight future research and innovation possibilities.

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# INVITED

**IL-1**

# Natural and Unnatural Phenolic Based Small Molecules: Green Chemical Synthesis and their Biological Evaluation

**Arun K. Sinha***

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Phenolics are a group of organic compounds with one or more hydroxyl groups on the aromatic ring and are widely distributed in plant kingdom. They range from simple phenols to complex compounds known as polyphenols. Interest in accessing these polyphenolics have gained pace because of plethora of biological activities such as anticancer, antibacterial, antifungal, anti-inflammatory and antimalarial etc. However, exploration of these phenolics is severely hindered by their insufficient percentage in their natural resources, difficult isolation procedure, limiting trials for wider applications besides their tedious synthesis involving protection-deprotection strategy. A protection/deprotection event introduces at least two steps into a sequence, incurring costs from additional reagents and waste disposal besides leading to a reduced overall yield. In this context, the concept of Green Chemistry has provided a fresh stimulus to develop a strategy with minimum number of steps, atom economy and waste minimization besides being devoid of protection-deprotection steps. For this various tools and strategies of green chemistry such as microwave/ultrasound-assisted reactions, ionic liquid, tandem reactions, cooperative catalysts, water-assisted reaction etc are being explored for the synthesis of various bioactive molecules including heterocyclic and phenolic compounds. Our group from noticeable time working on such green methodologies for synthesis of various phenolic based bioactive molecules like FEMA-GRAS approved 4-vinylphenols, stilbenoids (symmetrical/unsymmetrical, distyrylbenzene and octupolar stilbenes) and stilbene-chalcones/stilbene-cinnamate hybrids and their biological evaluation. The details will be discussed during presentation.

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**IL-2**

## A Small Focused Library of Diversely Functionalized Biodynamic Heterocycles

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In recent years, click chemistry has emerged as a fast and powerful approach to the synthesis of novel compounds with desired properties. The concept of "click chemistry" was coined by Sharpless to describe a set of "near perfect" bond-forming reactions which were very selective, high yielding, and wide in scope and describes chemistry tailored to generate substances quickly and reliably by joining small units together. 1,2,3-Triazoles are important class of target molecules due to their interesting biological properties such as anti-allergic, anti-bacterial, and anti-HIV activity. We were encouraged to combine 1,2,3-triazole moieties with phenol, coumarins, isatin, benzthiazinone, acetophenone, quinoline, 2,4-thiazolidinedione and acid hydrazide in a single molecular framework.[1] In addition to this, we have synthesized a library of thiazolidinone, thiazolidinedione and rhodanine incorporated highly functionalized molecules *via* green chemistry approach.[2] All the diversely functionalized molecules were synthesized from commercially available starting materials in minimum steps with high overall yield and screened for antitubercular, antioxidant, antimicrobial, anti-inflammatory and cytotoxic activities and will be discussed.

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**IL-3**

## Preclinical Toxicity Assessment of RISUGadv as A New Molecule for the Prevention of Prostate Cancer in India

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**Abstract:** The aim of this study was to assess the toxic effect of the newly innovated molecule - RISUGadv in male Charles Foster rats. Young and healthy male rats of Charles Foster strain were employed in the study. They were randomly assigned to two groups, control and treated, each consisting of fifteen animals. The new molecule RISUGadv was injected surgically in the vas deferens of the anesthetized control and treated group rats, respectively and observed for a period of 14 days. Initial and final body weights and food/water consumption of the animals were recorded. The haematological and biochemical parameters were analyzed. At the end of the study all the animals were sacrificed and necropsied, the organ weight was taken and their histopathological slides were prepared for microscopic examination. Body weight, food and water consumption, haematology, biochemistry, absolute and relative organ weights did not show any significant change and were well within the limit of normalcy. General health check-up, mortality, gross and microscopic examination of organs and tissues also did not reveal any sign of toxicity. From the toxicity point of view, this newly innovated molecule RISUGadv does not have any adverse effect and is safe to use.

**IL-4**

## New thoughts in drug research to prevent teratogenicity

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Animals and human get many of the same illnesses. Medical research with animals is one type of medical research, but other types include experiments with cells and chemicals and simulations on computers. Animal research usually describes research involving vertebrates, such as cats, mice, frogs, pigs, and primates. All medical research is carefully planned, and this includes medical research with animals. Under federal law, all animals must be treated humanely and undergo the least distress possible.

Medical research with animals saves Lives. Dog- discovery of insulin, monkey-- polio vaccine, mouse-- rabies vaccine, pig ---skin grafts for burn victims and computer-assisted tomography (CAT) scans, rabbit-- corneal transplants, rat--carcinogen screening. Medical research that helps animals discovery how it helps animals research on viruses, for example dog--- parvo virus vaccine.

In late 1950's and early 1960's the drug Thalidomide caused an estimated 10,000 birth defects and thousands of fetal deaths worldwide. The affected babies typically suffered from phocomelia, a failure of the limbs to develop. These unfortunate babies were cruelly referred to as "Flipper babies".This drug formerly used as a sedative, but with drawn in the early 1960's after it was found to cause congenital malformation or absence of limbs in children whose mothers took the drug during early pregnancy.Thalidomide is a sedative that used to be prescribed to treat anxiety, tension, gastritis and insomnia.It was also used to relieve morning sickness in pregnant women.

Man today living in a world created by him that is becoming more and more hostile every day owing to pollution. The subtle effect of Thalidomide tragedy resulting in phocomalia, apoda etc. in the offspring led to untold miseries. There are similar good number of cases of fetal deaths, still births, teratogenices etc. the young ones of mothers exposed to toxic ants like pesticides, radiation, heavy metal etc. Can we save innocent lives was the question that was prompted me to choose the topic of my research. Doing research with human subjects is illegal and unethical. So I have to go non-human material which stimulates human being. To study the long term effects of the toxic-ants on the fetal development. Rats have 21, rabbits 30, dog has 60 days gestation period. Whereas gestation period is long as in case of sheep, monkeys, elephants,they are not available because of cost procurement and maintenance. So in this situation scorpion comes handy, cheap, available, viable and reliable, with viviparity and long gestation period .All scorpions have a long gestation period. It goes from several months to a year and a half, depending on species. The young scorpions develop as an embryo in the mother's uterus. During this time, the embryo gets food from his mother. Hence scorpion was chosen as a medical research model. It is found in my research; by administering the chelating agents like Dimercaprol (BAL) to the heavy metal exposed mothers the adverse effects of Mercury and Lead on both mother and the fetus could be elevated.

**Objectives:**

The known drugs that more or less cause teretogenecity , Methamphetamine,Thalidomide, Isotretinoin (used in treatment of cystic acne), Methotrexate (Folic acid antagonistic) Azathioprine (renal transplant), Cyclophosphamide (infant malformation), Chloroquine (cochlea vestibule perisis) Phenytoin, valproic acid, carbamazine (cleft palate,congenital heart disease), Lamitrigine (increased

malformation risk), Propylthiouracil (cross placenta and may cause fetal goiter), Benzodiazepine (fetal benzodiazepine syndrome), Trimethoprime (increased risk of birth defects ), Tetracycline, Streptomycin, Kanamycin (brown discolorization of teeth, ototoxicity ),Cotrimazole, miconazole (Risk of abortion), Fluconazole (risk of limb deformities) etc.

This can be summarized as:

1. New thoughts in drug research to prevent teratogenicity.
2. New biochemical targets for drug screening
3. The research work focuses on drug discovery
4. Why more failures than success?

**The proposed Lecture covers:**

1. **Provocation**--- These are the challenging areas where basic scientists and clinicians need to have cross link. There are several drugs candidates that were successful in animal model but failed in clinical trials.

2. **Cogent--Fecund**--The present talk has diversified interests in focusing both basic and clinical aspects of drug discovery. The talk focuses not only on drug discovery also on novel path ways to be targeted in drug research , animal models, and also hot debate on failure and success of drugs. Thus this talk has a great scientific coeur, adoucissement, and attenuation for basic researchers and clinicians.

IL-5

# Carbocyclic nucleosides: A potential scaffold in Antiviral Drug Discovery

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**Abstract:** Mimetic based discovery yielded several promising drug candidate in past. Carbocyclic nucleosides have a potential to behave as a nucleoside mimetic and shown promising therapeutic efficacy as antivirals. The diverse exploration of carbocyclic nucleosides is limited due to their synthetic difficulties. The generation of new base and modified carbocyclic sugar is the key strategies to yield a novel carbocyclic nucleoside. The carbocyclic nucleosides can provide conformational preference to achieve better nucleoside mimetics as antiviral drug candidate. Regioselective synthesis of pyrazolo[3,4-*d*]pyrimidinebasedcarbocyclic nucleosides using cyclopentene sugar key intermediateexplored for antiviral evaluation.QM and MM based investigation provides the theoretical basis of regioselectivity followed by NOE and UV studies to confirms the selectivity. The carbocylic nucleoside conformation, binding mode and drug like properties are major determinant for potential mimetic. It was found that halogen in carbocyclic nucleoside has a special role to demonstrate significant anti-hepatitis activity. Unnatural stereochemistry exploration in carbocyclic further opens a scope fornew antiviral development.*(Authors thanks to DST, India for financial support.)*

**IL-6**

## Nano-antibiotics for Enhancing Treatment of Bacterial Infections

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Bacterial infections, associated with several infectious diseases, and which also play a role in the development of non-communicable diseases such as cancer and cardiovascular conditions remain a major threat globally. Challenges in addressing this problem are compounded by the current global crisis of bacterial resistance to antibiotic drugs. There is a rapid rise in the use of nanotechnology for the delivery of antibiotics via nano-sized drug delivery systems (NDDS) instead of conventional dosage forms as an approach to enhance antibiotic delivery and eradicate microbial resistance. Advantages of NDDS include targeted and uniform drug distribution in the target tissue, enhanced cellular internalization and sustained drug release, which improves efficacy, minimizes side effects, decreases administration frequency and improves patient-compliance. Most importantly, it has been reported that NDDS have the ability as a delivery system itself to overcome various drug resistance mechanisms by microbes. Whilst extensively studied for disease conditions such as cancer, the design and evaluation of NDDS for antibiotics to maximize treatment of bacterial infections is still in its infancy. This presentation will highlight various NDDS developed in our laboratories including nanoplexes, silver nanoparticles, dendrimers, lipid-dendrimer hybrid nanoparticles, pH responsive liposomes, and solid lipid nanoparticles for effective treatment of infections by *Staphylococcus aureus*and MRSA. Their preparation and physicochemical/biological/in silico/in vitro and invivo properties will be highlighted.

IL-7

## Tight Integration of Pharmacokinetics and Pharmacodynamics in the Design of Leads - A Case Study

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**Abstract**: We will present the potential of an*in* silico *approach* for minimizing attrition of leads in the later stages of drug development. We propose an approach, wherein 'parallel' information is generated to simultaneously optimize both the pharmacokinetics (PK) and pharmacodynamics (PD) of lead candidates. As a test case we consider the β-blockers, though in use for many years, have suboptimal PK. This approach utilizes molecular modeling tools *viz*. hologram quantitative structure activity relationships, homology modeling, docking, predictive metabolism, and toxicity models. Validated models have been developed for PK parameters such as volume of distribution (log $V_d$) and clearance (log Cl), which together influence the half-life ($t_{1/2}$) of a drug. Simultaneously, models for PD in terms of inhibition constant $pK_i$ have been developed. Thus, PK and PD properties of β-blockers were concurrently analyzed and after iterative cycling, modifications were proposed that lead to compounds with optimized PK and PD. We report some of the resultant re-engineered β-blockers with improved half-lives and $pK_i$ values comparable with marketed β-blockers. These were further analyzed by the docking studies to evaluate their binding poses. Finally, metabolic and toxicological assessment of these molecules was done through *insilico* methods. The strategy proposed herein has potential universal applicability, and can be used in any drug discovery scenario; provided that the data used is consistent in terms of experimental conditions, endpoints, and methods employed. Thus the 'parallel progression approach' helps to simultaneously fine-tune various properties of the drug and would be an invaluable tool during the drug development process.

**IL-8**

## Applications of NMR spectroscopy for Serendipitous Chemistry

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**Abstract:** Nuclear Magnetic Resonance Spectroscopy is one of the important techniques for determining chemical structures of natural products and synthetic compounds. Over the 35 years, NMR spectroscopy demonstrated tremendous impact on organic chemistry and biomolecular structure determination in all stages of drug discovery and development. With advances in NMR spectroscopy, complex structures can be solved with much less than 1 mg of compound. In continuation of our drug discovery program, we applied this modern tool to identify the novel chemical structures from nature and also unexpected products formed during the synthesis of natural products and their analogues, which resulted in the development of new chemistry will be discussed.[1-7]

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**IL-9**

# Acetal with Hydroxylactam: New Collaboration in Asymmetric Catalysis

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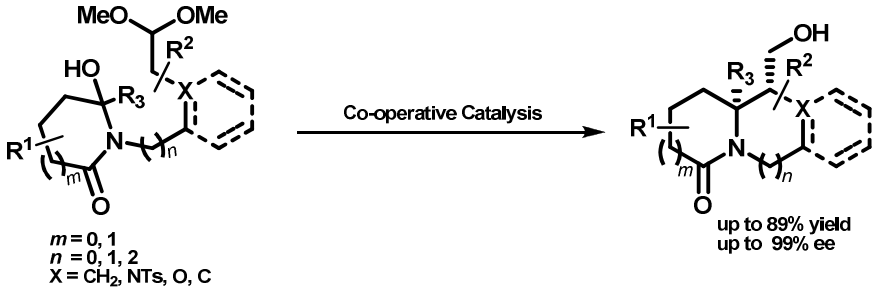
**Abstract:** Asymmetric organocatalysis[1] has been demonstrated as a powerful strategy for the synthesis of optically pure compounds from simple achiral precursors. Several otherwise impossible transformations have been documented in the last decade. Despite notable progress in implementing various transformations, strategy that exploits biosynthetic pathway to synthesize bioactive natural products and/or natural product like molecules using organocatalyst is less common.[2] However, this strategy would allow the enantioselective synthesis of bioactive natural products and/or natural product like scaffolds in step-economic way.

Following a biosynthetic pathway, we have very recently developed[3] organocatalytic enantioselective acyl-Mannich cyclization that furnishes bicyclic alkaloids which lead to the synthesis of bioactive natural products and natural product like molecules. Herein, we would like to present our recently disclosed novel approach that uses acetal and hydroxylactam (both derived from aldehyde) as pro-nucleophile and pro-electrophile, respectively, via co-operative organocatalysis for the synthesis of bicyclic alkaloids.

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**IL-10**

## Natural products-inspired discovery and development of anti-microbial, anti-inflammatory and antiplatelet agents

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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.). Several of these compounds 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, acetyl 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 at the ISCB Conference.

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**IL-11**

## Current Challenges in affordable and sustainable drug discovery from traditional Indian medicine

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"Until man duplicates a blade of grass, nature can laugh at his so-called scientific knowledge. Remedies from chemicals will never stand in favour compared with the products of nature, the living cell of the plant, the final result of the rays of the sun, the mother of all life." - T. A. Edison

Mankind was, is and will be depending on nature derived pharmaceuticals for all their health needs. There is increasing use of herbal formulations from traditional systems of medicine worldwide. When entering a pharmacy today, considerable shelf space is devoted to herbal formulations to a degree which would have been quite unimaginable even 20 years ago. The market value and economic value of herbal formulations is ever growing. In India the herbal formulations are playing a major role in our national health care system and its contribution for our economy is ever increasing.

The natural plant products often serve as chemical models or templates for the design and synthesis of new drug entities/ novel phyto-constitutents. For example atropine, quinine, physostigmine, cocaine, morphine, codeine, benzocaine, procaine and salicylic acid have served as a model for design and synthesis of anti-cholinergic, anti-malarials, anti-cholinesterases and local anaesthetics.

The growing concern in the recent past over the toxic effects of various synthetic drugs has forced the researches, academicians and doctors to consider some steps for discovery of novel phytoconsituents from herbs used as medicine. The occurrence of side effects after a long term use of synthetic drugs is always feared during the treatment of chronic diseases hence plants continue to be important sources of new drugs/novel phytoconstitutents with comparitively less side effects, as evidenced by the recent approvals of several new plant derived drugs and synthetic drugs based on secondary plant metabolites. Etoposide is a new semi-synthetic anti-neoplastic agent derived from *Podophyllum peltatum* has been reported to be useful in chemotherapeutic treatment of refractory testicular carcinomas, small cell lung carcinomas, non-hodgkin's lymphomas and nonlympholytic leukemias.

In the last two decades, the scientific community has shown a fast increasing interest in pharmacognosy and natural products research especially in the discovery of novel Phytoconstitutients from the Indian system of Medicine. The future of phytopharmaceuticals is bright as it, undoubtedly, serves as a cheap and steady source for varied range of therapeutic agents which are of great significance in the health care of mankind.

Today the major problem faced by the scientific community is establishing the quality of herbal drugs. The problems specific to the quality of herbal drugs are selective analytical methods may not yet exist, reference compounds may not be available commercially, adulterant and substitution and Biological variation such as Chemical and Natural variation / biodiversity Chemovarieties (e.g Thyme ) and Chemocultivars (e.g. Chamomile).

The long term benefits of herbal formulations outweighs the other forms of medicines and novel phytoconstituents are today emerging as more reliable medicine both scientifically and clinically. The novel Phytoconstituents will transform the health landscape of India and play a major role in achieving "Health for all".

"All that man needs for health and healing has been provided by God in nature, the challenge of science is to find it." Philippus Theophrastrus Bombast that of Aureolus ~ Paracelsus (1493-1541)

**IL-12**

# Sugar-modified Nucleosides and Sugar-based Amphiphiles as Nanocarriers

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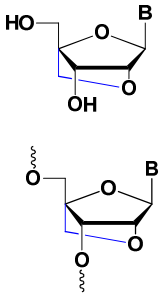
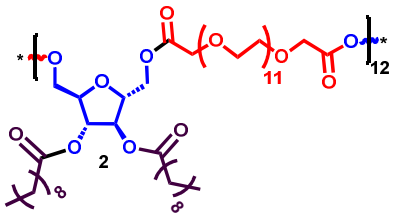
The use of biocatalysts in the modification of sugars has become an attractive alternative over conventional chemical methods due to their selectivity and high efficiency. We have successfully used lipases for the synthesis of sugar modified bicyclic nucleosides. Further, we have used the modified sugar precursor for the synthesis of amphiphiles, chiral crown ether analogs and corresponding [2]pseudorotaxanes.

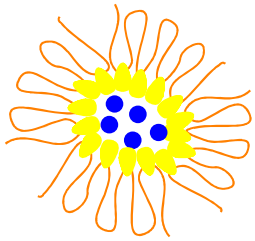



PEG 600

50 % acylation

C-10 alkyl chain



**LNA-monomers** **[2]pseudorotaxanes** **Drug Nanoformulation**

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IL-13

# Base-Mediated and Protection Free [4+2] Cycloadditions of Alkynes with Azadienes: An Efficient Assembly of Functionalized Quinolines

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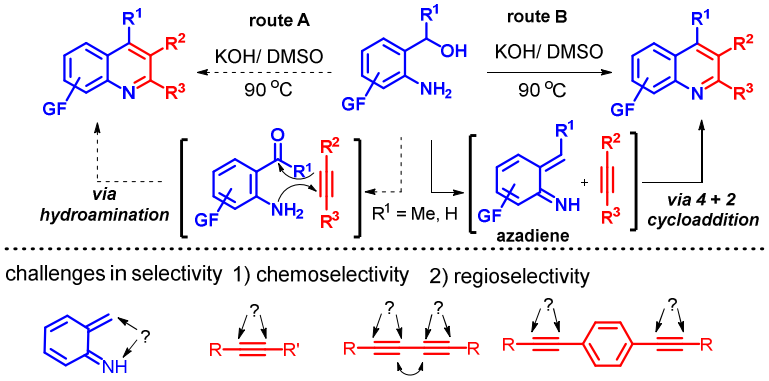
The [4+2] cycloaddition reaction is among the most powerful tools for generating carbocycles[1] and *N*-heterocycles,[2] it is often difficult to form systems that are highly congested or possess substituent arrays that are incompatible with the reaction. A literature survey revealed that metal and protection-free, base promoted intermolecular [4+2] cycloaddition for the synthesis of quinoline remain elusive. In continuation of our ongoing research on the base-mediated reactions[3] and *N*-hetreocyclic synthesis,[4] in this presentation I would like to discuss about our recent success on base promoted metal and protection-free synthesis of highly functionalized quinolines from *in situ* generated azadiene and internal alkynes via [4+2] cycloaddition process with an excellent chemo- and regioselectivity.[5]

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IL-14

# Synthesis of Thio/Seleno Ethers and Esters Under Metal Free Conditions *via* C-H Functionalization

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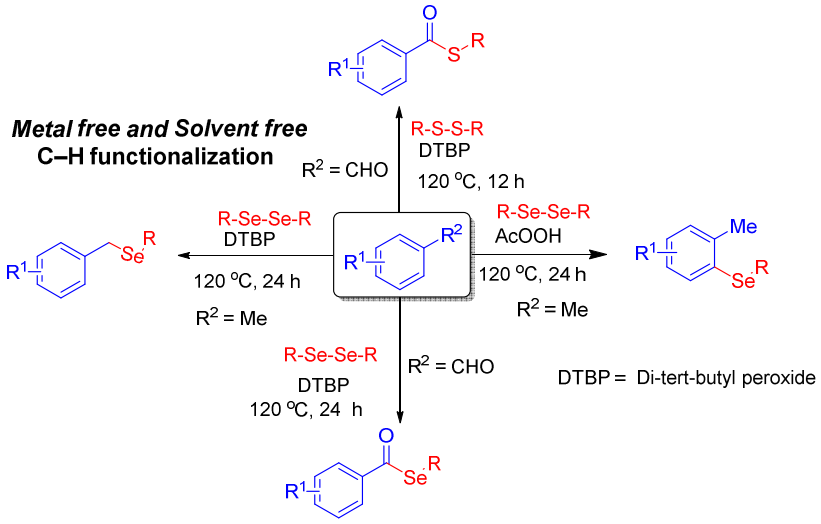
**Abstract:** Recently, the metal free organic transformations especially *via* peroxide catalysis emerged as interesting substitute for the metal catalysed coupling reactions. Various C-C, C-S, C-N, C-O, C-Se bond forming reactions have been carried out under peroxide catalysis.[1] These reactions proceed via radical mechanism. An Oxidant dependent metal free and solvent free thiolation/selenation of methyl arenes/aldehydes using disulfide/diselenides as source of sulphur/selenide has been described. The resultant thioether, selenide ethers, thioesters were obtained in good to excellent yield.[2]

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IL-15

# Molecular hybrid based drug design: A lesson from the nature

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The design of new molecules with improved ADME properties along with effective pharmacological potency; lack of toxicity and devoid of resistance for the treatment of infectious diseases has remained a big challenge for the scientific community. In order to address these issues concept of hybrid molecules was put forward which deals with the covalent hybridization of two or more distinct pharmacophores into a single molecule that may lead to a hybrid molecule with improved efficacy [1-3]. This approach may solve the problem of drug resistance and reduce the undesired side effects [4]. The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials. Towards these goals we have synthesized various molecular hybrids and tested these for antimalarial, anti-TB and anti-cancer activities and efforts will be made to present our recent work [5-22].

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**IL-16**

## Drug discovery strategies for the latent tuberculosis infection

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Cysteine has been implicated as an important amino acid in the redox defense of *Mycobacterium tuberculosis*, not at least as a building block of mycothiol. Several enzymes of cysteine biosynthesis have been shown to be essential for survival of the pathogen in infected macrophages, in particular for persistent *M. tuberculosis*. Potentially the pathways leading to *de novo* biosynthesis of cysteine provide suitable targets for the development of inhibitors that may be active against this pathogen also in the dormant stage of the disease. Here we report the identification and characterization of potent inhibitors of CysK1 and CysM, critical enzymes in the biosynthesis of cysteine during dormancy, based on e-pharmacophore and subsequent hit expansion. Biochemical binding and activity assays and three-dimensional structures of several enzyme-inhibitor complexes provided insights into mode of inhibition and enzyme-ligand interactions. The top compounds showed bactericidal potency in the low □M range against *M. tuberculosis*, with little or no cytotoxicity. Noteworthy several compounds displayed significantly improved potency in a nutrition-starvation model of dormancy when compared to first-line drugs such as rifampicin and isoniazid. Few of the compounds also showed in-vivo potency in M. marinum infected Zebra fish model.

**IL-17**

## Hybrid methods guide structure based vaccine design for picornaviruses

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The physical properties of viral capsids are major determinants of vaccine efficacy for several picornaviruses which impact on human and animal health. Current picornavirus vaccines are frequently produced from inactivated virus. Inactivation often reduces the stability of the virus capsid, causing a problem for Foot and Mouth Disease Virus (FMDV) where certain serotypes fall apart into pentameric assemblies below pH 6.5 or at temperatures slightly above 37°C, destroying their effectiveness in eliciting a protective immune response. As a result, vaccines require a cold chain for storage and animals need to be frequently immunised.

FMDV is a member of the Aphthovirus genus of the Picornaviridae. Globally there are seven FMDV serotypes: O, A, Asia1, C and SAT-1, -2 and -3, contributing to a dynamic pool of antigenic variation. We sought to rationally engineer FMDV capsids either as infectious copy virus or recombinant empty capsids with improved thermo-stability for improved vaccines. Here we used *in-silico* molecular dynamics (MD) simulations, molecular modelling, free energy calculations, X-ray crystallography, Cryo-electron microscopy and various biochemical/biophysical techniques to design and help characterise the improved capsids.For the most unstable FMDV serotypes (O and SAT2), panels of stabilising mutants were characterised by MD. Promising candidates were then engineered and shown to confer increased thermo-stability and pH-stability. Thus, *in-silico* predictions translate into marked stabilisation of both infectious and recombinant empty viral capsids.

An *in-situ* diffraction method was used to determine crystal structures for quality assessment and to verify that no unanticipated structural changes have occurred as a consequence of the modifications made. Where it was difficult to obtain crystals/diffraction, structures were determined by high-resolution cryo-electron microscopy. The structures of the wildtype and two of the stabilised mutants for three different serotypes of FMDV showed the mutations made predicted interactions and the antigenic surfaces remained unchanged.

Animal trials showed stabilised particles can generate improved neutralising antibody response compared to the traditional vaccines. Here, we have successfully used a structure based rational engineering approach to increase the stability of FMDV capsids without affecting the antigenic properties of the virus and demonstrated the direct application of structural biology and structure based design that has the potential to lead directly to a new generation of efficacious vaccines that can provide hope that the disease can be brought under control.

IL-18

## Intranasal Insulin: A Promising Treatment for Alzheimer Disease

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**Abstract**

Insulin/Insulin receptor signaling is involved in memory functions. Alzheimer disease (AD) is associated with reduced insulin level and impairment of insulin receptor (IR) signaling, which correlates to amyloid pathology and tau hyperphosphorylation in the brain. However, the molecular mechanisms associated with the beneficial effect of intranasal insulin on AD pathology are largely unexplored.Therefore, we investigated the effect of intranasal insulin in streptozotocin (STZ) induced memory impaired rats as evaluated in the Morris water maze test. STZ (ICV) treated group had shown memory impairment along with a decrease cerebral blood flow (CBF) (measured by laser doppler flowmetry). Intranasal insulin delivery significantly improved STZ induced memory impairment along with CBF in rats. STZ (ICV) induced a significant decrease in IR signaling molecules expression and ATP level in the hippocampus. STZ (ICV) injection also stimulates neuroinflammation (TNF-α, IL-10, & NFkB translocation), oxidative/nitrosative stress, cholinergic dysfunction, and apoptotic cell death in the hippocampus region of rats. Insulin treatment by intranasal delivery improved IR signaling molecules expression and ATP level and, attenuated neuroinflammation, oxidative stress, cholinergic dysfunction, and apoptosis in STZ induced memory-impaired rats. Also, intranasal insulin delivery successfully restored BDNF level and pCREB expression in STZ injected rats. Our findings reveal that insulin has the neuroprotective effect and supports the potential use of intranasal insulin delivery for the treatment of AD.

**IL-19**

## Identifying novel substances by creative use of value added databases

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There are several approaches one can take to identify new molecules or newer applications of the known moieties. One such approach is to leverage the value added databases consisting of published patents and journal articles.

During the process of drug discovery, many possible drug candidates are either suspended or discontinued due to reasons like toxicity, failed clinical trials or commercial reasons. A close analysis shows that the new derivatives of these discontinued drugs continue to get reported in literature as well as patents for similar or newer applications.

In most patents, claims cover the main scaffold along with variety of substituents in a generic manner. In addition specific examples are also given in claims as well as disclosure.

Intellectual analysis of these patents shows that there can be candidates which are not specifically mentioned in the patents. This brings possibilities to further explore derivatives of candidates or new substances that are structurally close using algorithms.

In this case study, we would present how value added databases bring up ideas for possible novel candidates and their synthetic approaches.

**IL-20**

# Synthesis of Bioactive Heterocyclic Compounds*via*Carbon-Hydrogen and Nitrogen-Hydrogen Bond Activation

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Nitrogen-containing heterocyclic compounds hold a special place among molecules of importance in pharmaceutical and biological chemistry.[1]Development of methods for these heterocyclic compounds, especially *via* C–N bond formation has been a research area of considerable importance.Encouraged by the progress made in the development of new transformations *via* carbon-hydrogen (C–H) and nitrogen-hydrogen (N–H) bond activation in recent years,[2]we explored transition metal catalyzed C–C and C–N cross coupling reactions based on C–H/N–Hbond activation for the synthesis of novel heterocyclic compounds.[3] The lecture will highlight protocols developed for the synthesis of some bioactive fused heterocyclic compounds starting from simple substrate employing C-H/N-H activation, tandem and multicomponent reactions (Figure 1).

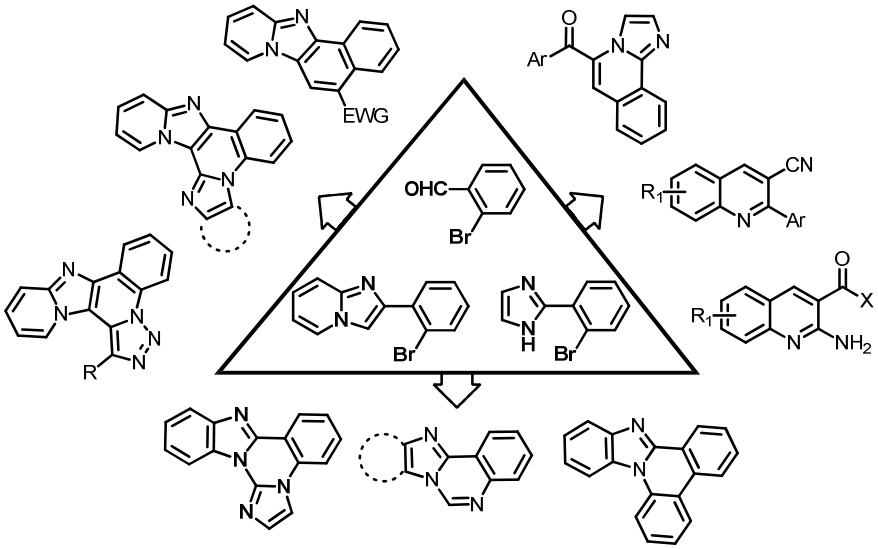


**Figure 1**: Synthesis of some bioactive fused heterocyclic compounds

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IL-21

# Metabolic variability among different accessions of guggul (*Commiphora wightii)* using GC-MS, HPLC and NMR spectroscopy

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*Commiphora wightii* (Arn.) Bhandari (syn. *Commiphora mukul*), commonly known as guggul is one of the most valued medicinal plants having several pharmaceutical applications. Guggul-gum is known from centuries to be efficacious in the treatment of rheumatoid arthritis, obesity, neurological diseases, hemorrhoids, urinary disorders, skin diseases and allied disorders, besides having other therapeutic uses. Guggul gum-resin has been extensively investigated for the presence of two ketosteroids, E-guggulsterones and Z-guggulsterones, the geometrical isomers (cis and trans) of pregna-4,17(20)-diene-3.16-dione are naturally occurring hypolipaemic agent which are present in stem resin of the plant. Fifty five accessions of guggul were collected from Ajmer, Barmer, Jaipur, Jaisalmer, Jodhpur and Udaipur, Rajasthan, India and were screened for their guggulsterone E and Z contents. Guggulsterone E and Z were quantified using RP-analytical HPLC. Guggulsterone E and Z varied greatly among the 55 accessions investigated. Guggulsterone Z content ranged from 5.46 mg to 22.17 mg $g^{-1}$ of dried latex, the lowest being in Rajgarh, Ajmer and the highest in Fatehsagar, Udaipur with an average of 11.6 mg $g^{-1}$ dried latex. Elite individuals with exceptionally higher guggulsterones content were identified. Non-targeted NMR and GC–MS based metabolomics approach was applied to profile aqueous and non-aqueous metabolites of three selected accessions of *C. wightii* in order to identify all the metabolites so that potential application for dietary supplements or nutraceuticals could be explored. Univariate and multivariate analyses were used for understanding and establishing the diversity of *C. wightii*. The NMR and GC–MS based non-targeted metabolite profiling identified 132 chemically diverse metabolites from non-aqueous and aqueous extracts of leaves, stem and latex of three different accessions of *C. wightii*. Non-targeted metabolite profiling of *C. wightii* resulted remarkable differences in the levels of various biologically active metabolites amongst chemotypes suggest that each part of particular chemotype can be use as potential medicinal supplements in healthcare industry.

**IL-22**

## Nitric Oxide Synthase (NOS) Inhibitors: Past, Present, and the Future

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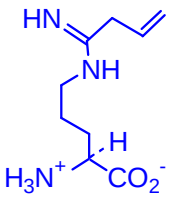
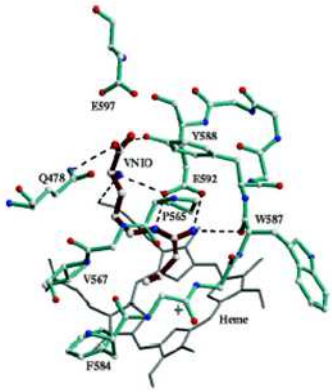
Nitric oxide (NO) is one of the smallest signaling molecules generated in mammals by Nitric Oxide Synthase (NOS) catalyzed conversion from L-Arginine to L-Citrulline. Three highly distant isoforms of Nitric oxide synthases (NOSs), namely neuronal (nNOS or NOS1), inducible (iNOS or NOS-2), and endothelial (eNOS or NOS-3), generates nitric oxide (NO) from L-Arginine through an oxidation process involved with Molecular oxygen and NADPH. Various physiological roles are involved with NO including vascular tone in endothelial system, host-defense in immune system, and long-term potentiation and memory in neuronal system. In contrast to significant biological roles of NO, there are number of pathophysiological conditions associated with high or low levels of NO. Most notably, nNOS implicated in stroke, migraine, and iNOS related in septic shock, arthritis, and multiple sclerosis. Therefore, considerable efforts are expended in the development of isoform specific NOS inhibitors and designing such inhibitors based on amino acid (Vinyl-L-NIO) and non-amino acid (2-AMPT) type small molecules. The field was evolved and grown extensively in the past and significant contributions related to inhibitor-design and isoform-selectivity has been highlighted in the presentation along with new developments and future trends.

Amino acid-based NOS Inhibitors

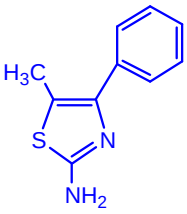



**Vinyl-L-NIO**

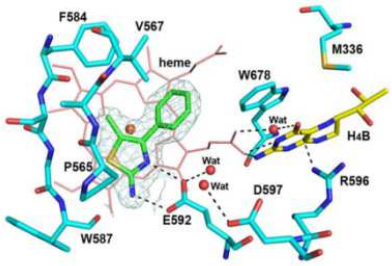



Vinyl-L-NIO with rat nNOS

Non amino acid-based NOS inhibitors




**2-AMPT**




2-AMPT with rat nNOS

**IL-23**

## Intellectual Property Rights; An Overview

**Vinay Tripathi**

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My lecture will cover Intellectual Property Rights along with its classification i.e. Patent, Industrial Design, Trade Marks, Copyright, Geographical Indications, Lay out Designs of Integrated Circuits, Trade Secret and Protection of New Plant Variety. Some of the important features of Patents Act 1970 & Patents Rules 1972 and the success story of India's drug industry along with case studies will also be discussed.

**IL-24**

## Aquatic antimicrobial peptides (AMPs): Natural templates for design new antimicrobial compounds

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Infectious diseases have no boundaries causing terrific health impacts, thus posing a long-lasting critical global problem. Forthe past few decades, antibiotics served as effective therapeutics for various pathogenic infections. However, excess and non-specific usage of antibiotics resulted in the development of various multi-drug resistant pathogens and they continue to pose increasing therapeutic challenges. Thus, it has become mandate to move towards a post-antibiotic era requiring development of novel therapeutics. In recent years, many antimicrobial peptides have been identified which exhibit a unique mode of action avoiding traditional drug targets. Antimicrobial peptides are naturally available innate immune molecules, being able to act directly on the bacterial pathogens but also involve as immune regulators. In particular, invertebrates and primitive vertebrates from aquatic environment represent a resource with plentiful antimicrobial peptides. Transcriptome analysis of freshwater organisms such as snakehead murrel, *Channa striatus* and giant prawn, *Macrobrachium rosenbergii*, revealed a wide range of antimicrobial peptides. During fungal, bacterial and viral infections, the expression of RNA transcripts of those AMPs was significantly up-regulated which emphasize their immunological roles during infections. Interestingly, most of these peptides followed a membrane disrupting activity which denotes that the pathogens could not develop resistance against those peptides. In addition, altering the sequences of few membrane-binding peptides showed remarkable antibacterial activity. Altogether, aquatic antimicrobial peptides act as natural templates for designing and development of novel antimicrobial therapeutics.

IL-25

# Greener syntheses employing carbon dioxide: An easy access for the syntheses of biologically potent scaffolds

**Devdutt Chaturvedi***

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**Abstract:** In recent years, development of novel synthetic methodologies have been attracted a great deal of attention for organic chemists around the globe, for the synthesis of structurally diverse biologically potent molecules. The advantages associated with these synthetic methodologies are lesser synthetic steps, use of cheaper and safer new alternatives, involves overall lesser reaction time, milder reaction conditions, and afforded high yields. Extensive efforts have been made by organic chemists around the globe and thus developed several kinds of new and highly efficient methods for the generation of various kinds of structurally diverse molecules of biological significance.

In recent years, carbon dioxide has been employed as a cheap and safe alternative eliminating the use of harmful reagents such as CO and $COCl_2$. Recently, carbon dioxide has frequently been employed as a green reagent in its various conditions and forms for the syntheses of structurally diverse biologically potent scaffolds employing diversity of starting materials, reagents and catalytic systems. In the present talk, we will focus some of our novel and efficient methods for the synthesis of biologically potent scaffolds.

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**IL-26**

# Amino Acids Chirons: Quest for Bioactive Alkaloids and Steroidomimetics

Priyanka Singh[a], Ritesh Singh[a], Rituraj Konwar[b] and **Gautam Panda[a,*]**

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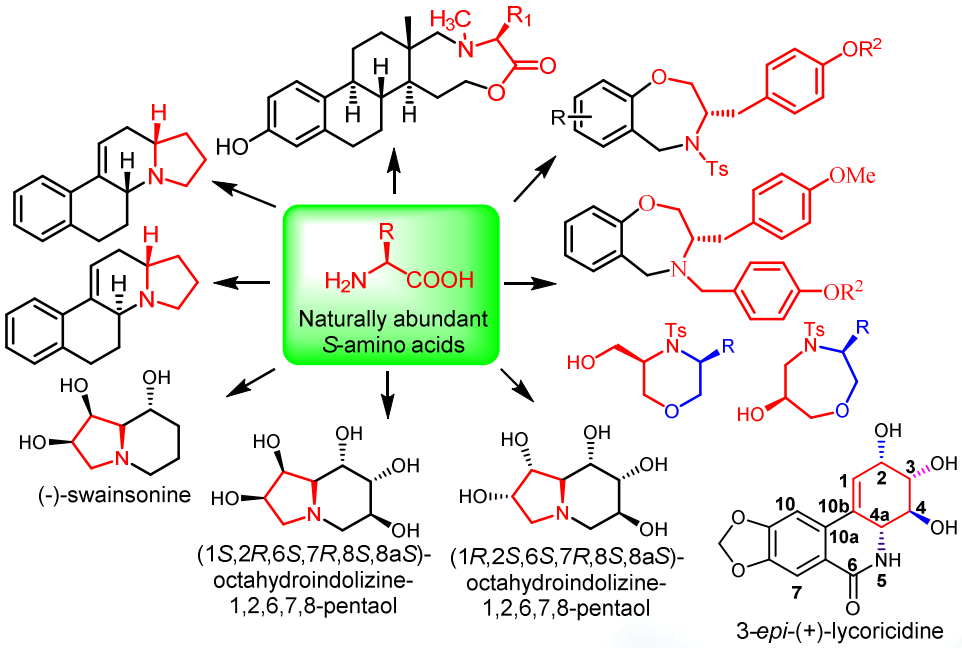
The amino acids have been utilized for the total synthesis of bioactive alkaloids having significant anticancer activity. Diastereoselective and diverse synthesis of polyhydroxylated indolizidines and piperidines have been described, where a common chiral intermediate 2-(hydroxymethyl) piperidine-3-ol is converted into (-)-Swainsonine, (+)-1,2-Di-epi-swainsonine, (+)-8,8a-Di-epi-castanospermine, Pentahydroxy Indolizidines, (-)-1-Deoxynojirimycin, (-)-1-Deoxy-altro-nojirimycin and related diversity. Amino acids can also be extended for the construction of steroidal and non-steroidal architectures in quest for steroidomimetics. Chirality derived from amino acid based architectures provides a new avenue to incorporate chiral chemical space within steroids which is otherwise obtained through several synthetic steps. The ring D of steroidal architectures can be mimicked with proline and phenyl group of amino acid tyrosine in quest for anti breast cancer agents. Diverse synthetic approaches along with their mechanism of action will be discussed.

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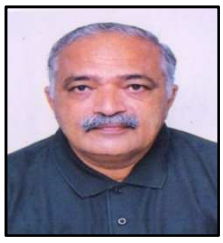
IL-27

# Landscaping of biological active of novel hybrid heterocyclic as antimicrobial, antitubercular and anticancer agents – A journey of one decade



**Nisheeth C Desai**

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The present talk focusses on the author's decade long research journey in the domain of synthesis and screening of biological activities of novel hybrid heterocyclic as antimicrobial, antitubercular and anticancer agents. Sheer perseverance and commitment helped the author and his research group publishes 25 research papers in the prestigious journalMedicinal Chemistry Research – Springer. The alarming rate of emerging and reemerging microbial threat of bacterial resistance has heightened the urgency to discover and develop effective agents with novel mechanisms of action and enhanced activity. Despite the development of several new antibacterial agents, their clinical value is limited in treating an increasing array of life threatening systemic infections.

Hence, the development of potent and effective antimicrobial agents is vital to overcome the emerging multi-drug resistance strains of bacteria and fungi. Also, there is great threat posed by the tuberculosis bacteria and current first-line tuberculosis drug treatment is more than forty years old, consisting of rifampicin and isoniazid. These antibiotics are drug-susceptible and require longer time and large number of doses, which are multi-drug resistant (MDR) and extensively drug resistant to tuberculosis strains. However, the rapid increase of multi-drug-resistant (MDR-TB) has led to an urgent need for the identification of new drug targets and the growth of novel anti-TB drugs.

In continuation to this author has focused on the synthesis of novel hybrid molecules using various medicinally important heterocyclic scaffolds such as, 1,2,3,4-tetrahydropyrimidine, quinazolinone, 1,3,4-oxadiazole, quinoline, 4-thaizolidinone, benzimidazole, 2-pyridone, 1,2,4-triazole, 1,6-dihydropyrimidine, imidazo-[1,2-α]pyridine, pyrazole, pyridine, pyrimidine, morpholine, imidazole, pyrazoline, thaizole, 2-azetidinone, cynopyridine. These molecular diversities are synthesized, characterized and screened for their antimicrobial, anticancer, antitubercular activities. Author has developed 450 molecular diversities for the publications.

IL-28

# Synthesis and Kinase Inhibition Study of Pyridylpyrimidinylaminophenyl Derivatives

**Sunil K. Sharma**

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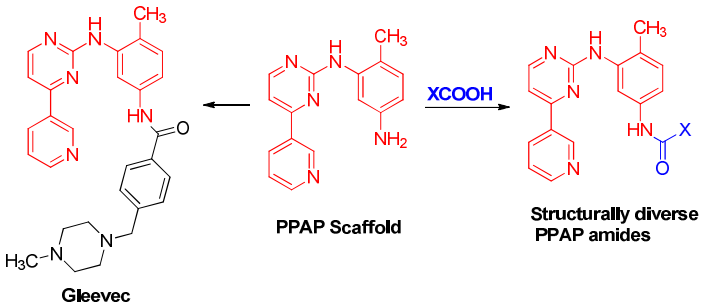
Deregulation of kinase activity has emerged as a chief mechanism by which cells evade normal physiological constraints on growth and survival leading to varied mortal diseases such as cancer [1]. The search for selective drugs for cancer treatment led to the discovery of Gleevec (Imatinib), the foremost FDA-approved tyrosine kinase inhibiting drug for treatment of chronic myeloid leukemia (CML) [2,3]. In continuation of our enduring research program in exploring, designing and synthesizing biologically active heterocyclic frameworks with antiproliferative and c-Src kinase inhibitory activities [4-7], we have designed and synthesized novel hybrid constructs and evaluated their kinase inhibition potential. Our synthetic approach is grounded on the rational concept of molecular hybridization, which has been exemplified as an effective tool for cogent design of novel molecular constructs by covalently conjugating two or more active pharmacophores [8]. The novel structurally varied amide/cyclic amide derivatives are hybrids of pyridylpyrimidinylaminophenyl amine the key pharmacophore of kinase inhibitor based drug molecule "Imatinib" [9] and shortlisted biologically potent heterocyclic acids. Kinase inhibition evaluation of various synthesized amides revealed one of the synthesized compound, a cyclic amide/pyridin-2(1*H*)-one derivative to be a potent candidate for kinase inhibition with $IC_{50}$ value quite comparable to the drug "Imatinib" against c-Src kinase. These synthesized analogs could serve as a gateway for developing next generation novel kinase inhibitors.

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IL-29

# A paradigm shift in natural product based drug discovery from classical to empirical approach

**Rakesh Rawal**

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**ABSTRACT:** Plants produce a huge variety of metabolites (metabolome) as a result of their interaction and adaptation to the environment. Mankind owes immense benefits from these plant metabolites for food, medicines, flavors and cosmetics. Phytopharmaceuticals, the drugs from plants and other natural compounds, since ancient ages are contributing towards human wellbeing and currently gaining momentum for the development of new medicines for several acute and chronic medical conditions including cancer. Many drugs listed as conventional medications are derived from plants and were originally administered in its native form. Rather than depending on in vitro and in vivo screens for antiproliferative activity, investigators can now focus on new molecular targets and pathways essential for the development and maintenance of the cancer phenotype. In the post human genome era globally investigators have explored the cancer genome and transcriptome which ended up with too many targets. Small bioactive molecules, obtained either from natural products or their semisynthetic derivatives or from synthetic chemical libraries, may be used as ligands to select and validate these array of protein targets. Therefore, the crux of cancer drug discovery lies in identification and validation of prime targets such that manipulation of the target function would cause some phenotypic or functional change in the cancer cell. Control of cancer would then only await the discovery of a drug molecule through a systematic screening and/or systematic drug design program. Approaches to target validation might involve the use of secondary metabolites screening using LC-MS or differential gene expression profile in response to phytopharmaceutical exposure. However, ultimate validation can only come from a successful clinical trial on cancer patients showing complete elimination of tumour, tumor shrinkage or significant change in a validated surrogate marker. Current presentation shares our experience and results obtained from in-vitro studies of several phytochemicals screened on cancer cell lines and in-vitro models derived from primary tumours.

**IL-30**

# Synthesis of N-glyconjugates and their applications in biological sciences

**Ajay K. Sah**

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Covalently sugar bound proteins lead to the formation of glycoproteins, which controls various life processes in the form of collagens, mucins, transferrin, immunoglobins, various hormones, enzymes, antifreeze proteins etc.[1] In most glycoproteins, glucose is covalently linked with a polypeptide unit *via* either O- or N-glycosylation.[1a,1b] Inspired from biological importance, we are engaged in exploring the synthesis and reactivities of N-glycoconjugates containing D-glucose and amino acids. Recently we have synthesized a series of N-glycoconjugates of D-glucose (Fig. 1) having amide-amide (**a-a**) and amide-imine (**a-i**) linkage.

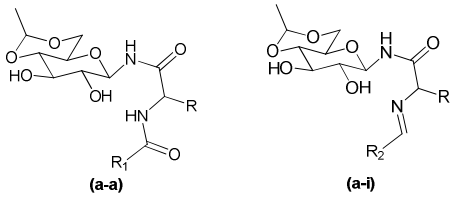


Fig. 1

One of the compounds of **a-a** series (N-(2-hydroxybenzoyl)-L-alanyl-4,6-O-ethylidene-*β*-D-glucopyranosylamine) has been used for molecular recognition of naturally occurring amino acids, and it selectively interacted with both the free and protein-bound tryptophan residues.[2] Six compounds of this series (Fig.2) have also been tested for anti-inflammatory and analgesic behavior.[3] On the other hand, twelve compounds of **a-i** series (Fig.3) have only been tested for antimicrobial activities.[4]

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# ISCB AWARDS

## ISCB Excellence Award 2017

# Extreme potency and selectivity in the design of inhibitors of the tankyrases, new targets in cancer and other diseases

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The poly(ADP-ribose)polymerase (PARP) superfamily of enzymes catalyse the transfer of one or many ADP-ribose units from $NAD^+$ to target proteins, regulating their activity. The archetypal PARP, PARP-1, is involved in the cellular response to DNA damage and regulates repair. It is the target of olaparib, an inhibitor recently approved for the treatment of BCRA-mutant ovarian cancer; other drugs are in late-stage clinical trial. The tankyrases (PARP-5a and PARP-5b) are isoform members of this superfamily. They are closely related to each other and have overlapping roles in regulating the length of telomeres, ensuring correct function of the mitotic spindle, transmission of proliferation signals in the Wnt / □-catenin system and in regulating the uptake of glucose into cells in response to insulin.

Using structure-based drug design, we developed a large series of 3-arylisoquinolin-1-ones, 2-arylquinazolin-4-ones and arylnaphthyridinones as inhibitors of the tankyrases. The diversity of substituents on these molecules allowed a comprehensive structure-activity relationship to be established. This led to identification of examples inhibiting tankyrase-2 (PARP-5b) with $IC_{50}$ in the low nM range and with selectivity >1000-fold *vs*. PARP-1 and PARP-2 (isoform-selectivity) and without effect on a $NAD^+$-requiring oxidoreductase, IMPDH. These inhibitors have been shown, in crystal structures, to bind as mimics of the nicotinamide moiety of $NAD^+$ and in an adjacent hydrophobic pocket and tunnel. More recently, we have developed new agents which bind at both the nicotinamide- and adenosine-binding sites, increasing potency ($IC_{50}$ = 100 pM, tankyrase-2) and selectivity (>$10^5$-fold *vs*. PARP-1). Cellular activity of these new inhibitors has been demonstrated in functional assays of Wnt / □-catenin signalling, pulmonary fibrosis and glucose uptake. The lecture will cover the development of these new super-potent inhibitors and expand on the broad range of potential therapeutic applications.

## ISCB Excellence Award 2017

# Fluorescent Molecules in Sensing and Imaging of Bio-analytes

**Ayyappanpillai Ajayaghosh**

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Small molecules with strong fluorescence have been extensively used as molecular probes for the detection of ions and neutral species in biological samples. Among different methods, fluorescence technique is preferred for sensing of analytes due to the high sensitivity of the signal. Therefore, a variety of fluorophores have been reported for the detection of biologically relevant analytes. In this context, we have been interested in the design of new fluorescent molecules and assemblies useful for the selective detection of biologically important cations,[1-4] neutral molecules,[5] imaging of biological samples and security applications. With this objective, we have reported a few fluorophores based on bipyridyl systems as sensors for the detection of $Zn^{2+}$ and cyanide ions.[6-10] Recently, we have demonstrated the used of fluorescent dye nanoparticles for the specific detection of BSA, HAS and pH of the medium.[11,12] Currently, we are working on new two and three photon active fluorescent probes for the sensing and imaging of zinc ions in biological samples.[13,14]

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## ISCB Young Scientist Award 2017

# Development in selective C-C bond formation: From Asymmetric Catalysis to C-H activation

**Ravi P. Singh**

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The relay of electronic effects through a conjugated organic bonding system, such as those in a vinylogous system provides opportunity to achieve transformation at a remote place. In this regard, vinylogous nucleophiles such as 2-silyloxy dienes (acyclic and cyclic) have emerged as powerful synthons. Particularly, 2-silyloxy furans useful in accessing γ-butenolides and γ-lactone frameworks have been extensively explored in the total synthesis of natural products and biologically active molecules. These heterocycles behave as a vinylogous nucleophile and after reaction with carbonyl and carbonyl derived compounds (aldehydes, ketones, aldimines, ketimines, enals, enones, and heteroatom-stabilized carbenium ions) offer a multitude of highly functionalized structures.[1],[2],[3]Also, it grants a synthetic track, where a number of functional group and selected stereochemistry can be established. In this presentation, a highly diastereo- and enantioselective organo catalytic asymmetric vinylogous Mukaiyama-Michael addition of various silyoxyfurans to enones,[4] and vinylogous aldol reaction of 2-silyloxyindoles to ketones which proceeds through the bifunctional catalysis,[5] will be presented. Also vinylogous Mannich reaction of a highly regio- and diastereo- selective TMSOTf promoted synthesis of chiral quaternary 3-aminooxindole butenolides from 2-silyloxy furans and chiral ketimines will be discussed.[6] Highly regio- and diastereo-selective Lewis acid catalyzed vinylogous Mannich reaction of 2-silyloxyindoles with chiral aldimines and vinylogous nucleophilic substitution reaction with diarylmethanols will be highlighted.[7]

As an example of selective C-H activation, a ligand enabled Cu catalysed intramolecular C-2 site selective Csp2-H/ Csp2-H activation method for *N*-substituted prrrole-azole system has been developed. Copper salts, comparatively economical than other transition metal salts and less toxic has also been used for intramolecular C–H coupling reaction between indole-2 and imidazole-2 moieties to deliver annulated polycyclic heteroarenes.8

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## ISCB Young Scientist Award 2017

# Rhodium Catalyzed Transannulation of *N*-Sulfonyl-1,2,3-Triazoles

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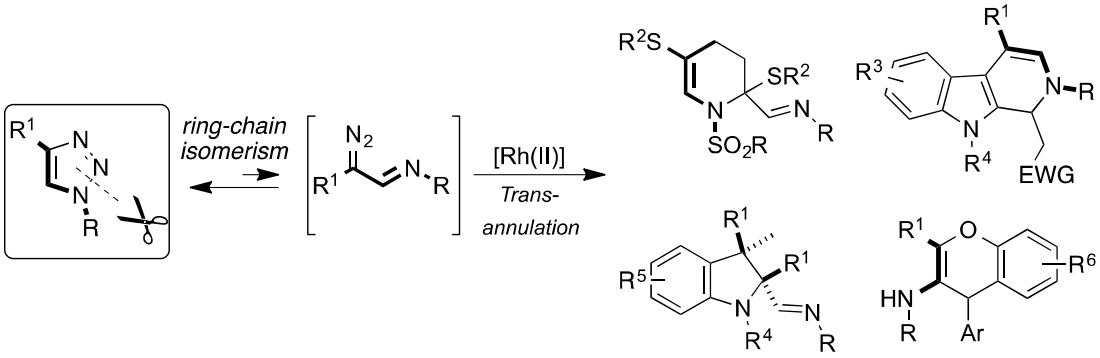
Transition metal-catalyzed functionalization of $\alpha$-diazocarbonyl compounds has found widespread application because of their ability to produce reactive metal carbene intermediates. These metal carbenes are capable of delivering variety of useful transformations,[1] which includes traditional reactions like cyclopropanation, X–(C)H insertion, ylide and contemporary reactions such as three component reactions. On the other hand, application of $\alpha$-diazoimines, nitrogen analog of $\alpha$-diazocarbonyl compounds in the above mentioned reactions are rather limited, due to its limited availability. However, the recent study on the 1,2,3-triazoles as source of $\alpha$-diazoimines opened a new avenue for diazo chemistry.[2] In this presentation, our recent efforts in the rhodium catalyzed denitrogentaive transannulation of *N*-sulfonyl-1,2,3-triazoles, *via* the generation of$\alpha$-diazoimines, to various nitrogen and oxygen based heterocycles will be discussed.[3]

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## ISCB Young Scientist Award 2017

# Proteostasis Restoring Factors: Molecular StrategiesAgainst Neurodegeneration and Ageing

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**Running Title:** *QCE3 Ubiquitin Ligases Confers Cytoprotection Against Proteotoxicity*

Cells continuously revive their physiological functions via replacement of old proteins in place of newly synthesized polypeptides. Efficient performance of Ubiquitin Proteasome System and Autophagy constantly eliminate deleterious accumulation of protiens from various cellular compartments. In cellular quality control system, E3 ubiquitin ligases are significant employees for defense mechanism against abnormal toxic proteins. Few findings indicate that lack of functions of E3 ubiquitin ligases can be a causative factor of neurodevelopmental disorders, neurodegeneration, cancer and ageing. However, the detailed molecular pathomechanism implying E3 ubiquitin ligases in cellular functions in multifactorial disease conditions are not well understood. This study systematically represents the unique characteristics, molecular nature, and recent developments in the knowledge of neurobiological functions of few crucial E3 ubiquitin ligases. Here, we present our recent finding on the roles of E6-AP, MGRN1 and ITCH E3 ubiquitin ligases in the neuropathobiological mechanisms, with precise focus on the processes of neurodegeneration, and thereby propose new lines of potential targets for therapeutic interventions.

**Key words**: *Misfolded Proteins; Neurodegeneration; E3 Ubiquitin ligases; Quality Control; Autophagy*

**Distinguish Women Scientist Award 2016**

# De novo tailored design of new metal-based drugs or drug precursors for antitumor chemotherapy: Structure elucidation by Single X-ray crystallography and their *in vitro* binding and cytotoxicity profile

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**Abstract:** Cancer is a complex class of disease inwhich a group of cells divide uncontrollably beyond thenormal limit, subsequently intruding to the near or distanttissues (metastasis), ultimately causing cell death. There are more than 100 phenotypes of cancers derived from numerous organs or tissues with multiple etiologies and endless combinations of genetic and epigenetic alterations. Therefore,**one**-drug-fits-**all** approach does not work for all the cancers. New tailored drug designstrategiesinvolving the specific site of action at the target site possessing lower systemic toxicity which could arbitrarily be done by choosingappropriate metal ion and tailoring ligand scaffolds as recognition elements and metal anchoring platform etc.

Considerable efforts are being undertaken for developing new drug entities/or through optimization of the drug protocols involvingcombination cocktails of present chemotherapeutic agents with a bioactive organic pharmacophore. Targeted cancer therapy involves the use of drugs or other natural compounds that block the growth and spreadof cancerous cells by interfering with specific molecules or pathways that are involved in cancer growth or progression. Many natural products like chromones and flavonoids etc. are considered to be privileged ligand scaffolds in medicinal chemistry that involve different types of cancer targets, viz. nucleic acids (DNA/RNA), enzymes (kinase inhibitors and topoisomerases), membrane receptors (dopamine D2 receptor agonists) etc.

In continuation to our previous interest of designing new tailored drug candidates for antitumor chemotherapy, we have carried out synthesis of a few notably important metal-based drug entities 1)Chromone-appended Cu(II) drug entity[$C_{36}H_{50}CuN_8O_6$] 2) ionic Sn(IV) iminodiacetic acid–piperazinediium conjugate[$C_8H_{17}N_3O_4Cl_4Sn$]3)**3)**Antitumor tetranuclearstannoxanecluster**,**$C_{24}H_{38}Sn_4Cl_2O_8$with exceptionallyhigh activity towards pancreatic cell line.4)Ag(I)nalixidic acid-piperazinediium complex 5) Enantiomeric L/D- phenylalanine derived Cu(II) conjugates [$C_{21}H_{22}CuN_4O_7$ ].Herein we will discuss their structure elucidation, *in vitro* DNA binding and cytotoxicity profile.

**ISCB Life Time Achievement Award 2017**

# HIGHLY EFFICIENT SYNTHETIC STRATEGIES FOR BIOACTIVE HETEROCYCLIC MOLECULES

**Prof. Murlidhar S. Shingare**

*Emeritus Scientist (CSIR), Department of Chemistry Dr. Babasaheb Ambedkar Marathwada University, Aurangabad - 431004.*
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The remarkable ability of heterocyclic nuclei has largely contributed to improve the lives of human beings. Though the heterocyclic molecules present in nature are large in numbers, their amount is not sufficient to fulfill the requirements of the overcrowded world of increasing demands. Therefore, the synthetic chemical community has been under increased pressure to produce these myriad of substances following efficient as well as greener synthetic strategies.

The diverse nature of the world of chemical synthesis requires various greener synthetic pathways in our quest towards attaining sustainability. One of the thrust areas for achieving this target is to explore alternative efficient reaction conditions to accomplish the desired chemical transformations with minimized by-products or waste and without the use of conventional volatile organic solvents, wherever possible. Consequently, several newer synthetic strategies have been appeared, such as reactions in greener solvents like water, reactions under solvent-free (dry media) conditions, mechanochemical mixing (grinding), use of solid-supported reagents. Apart from this, utilization of alternate heating and activation methods that employ microwave (MW) and ultrasonic irradiations for the rapid syntheses of organic molecules are also prominent. Availability of these efficient and greener synthetic alternatives, encourage us to explore its applications for achieving large number of organic transformations.

In consideration of the ever increasing biological/pharmaceutical significance of bioactive heterocyclic molecules, there is a need to continue the research for the development of these heterocyclic moieties by developing highly efficient and environmentally benign protocols. From the view point of sustainability, attempts should also be directed towards the exploitation of catalytic applications of easily available and inexpensive reagents for the synthesis of such bioactive heterocyclic molecules.

# ORAL

**O-1**

# Ugi Multicomponent Reaction and Insilico Study of Fluorinated carboxamides derivatives as an anti-tubercular agents

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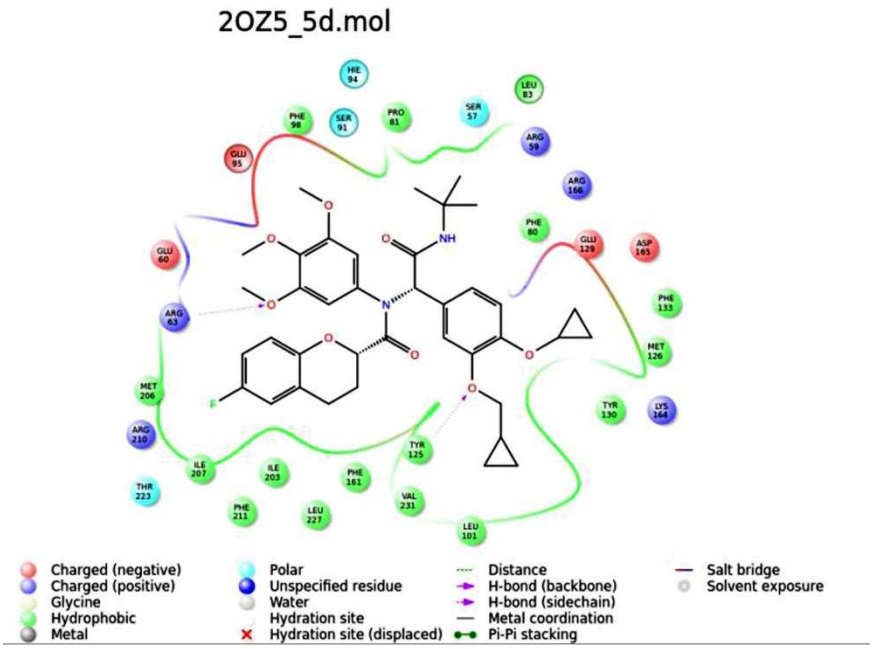
The carboxamides derivatives of flouro substituted chromane-2-carboxilic acid have been synthesized via Ugi four-component condensation (U-4CCRs) between 6-fluorochromane-2-carboxylic acid, various aryl aldehyde, 3,4,5-trimethoxy amine and *tert*-butyl isocyanide, to give *N*-((*tert*-butylcarbamoyl)(4-substitutedphenyl)methyl)-6-fluoro-*N*-(3,4,5-trimethoxyphenyl) chroman-2-carboxamide.The molecular level insights of all compounds were determine by molecular "**in silico"** study against the receptor tyrosine phosphatase PtpB. In the receptor active pocket with one and/or more amino acid, compounds show sound establishment. All these synthesized compounds were screened for their anti-mycobacterial activity against *Mycobacterium tuberculosis H37Rv* to determine the Minimum Inhibitory Concentration (MIC) at different level such as $IC_{50}$ and $IC_{90}$.




By evaluation of docking results, compound **5d**, was considered to be the potent inhibitor, which gave strong supportive coordinate to the in vitro study. It is highly active against *H37Rv*, having MIC and $IC_{50}$ value of was 70 µM and 53 µM respectively in vitro study.

**O-2**

## Identification of Novel Drug Targets through subtractive genomics approach

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Target identification is an initial step in the drug and vaccine discovery process. Various methods are adopted to identify novel drug targets depending on the type of disease. The transcriptome and proteome data of an organism can be analysed in the case of non-communicable disease and thesubtractive genomics approach is found effective in the communicable disease. In the recent years, a large number of novel drug targets have been identified for bacterial and fungal pathogens that are either drug resistant or for which no suitable vaccine is available. This approach reduces the time as well as the cost of drug target screening. As it is a computational approach, many pitfalls are there in the analysis and interpretation of the data. The current talk emphasises on the methods and numerous available tools and databases to identify novel drug targets. Also, it provides both merits and demerits of the technique with suitable example.

**Keywords:** BLAST, Similarity, Orthologous, DEG, Drug Target

**O-3**

## Natural product and its derived compounds as a source of new lead in drug discovery

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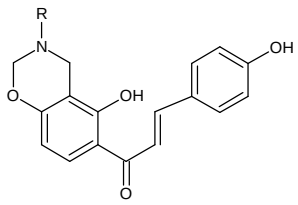
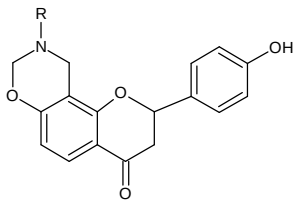
Malaria is still the most destructive and dangerous parasitic infection in several tropical, subtropical countries. The impact of this disease is getting worse, due to the increasing resistance of *Plasmodium falciparum* against available antimalarial drugs. There is an urgent need for new, more affordable, accessible antimalarial agent. Natural products have played important role in the discovery of leads for the development of drugs to treat human diseases, hence new antimalarial leads may certainly emerge from tropical plant sources. In order to find out more potent phytomolecules from plants, in our study we have selected five Indian medicinal plants viz. *Cleome gynandra, Sesbania grandiflora, Mikania micrantha, Glycyrrhiza glabra, Polyalthia longifolia*. These plants have recently shown good biological activities, so our main focus is on isolation of the compounds responsible for anti-infective activity of these plants. Extraction of different parts of the plant has been done separately, plant extracts and isolated molecules are submitted for biological activities.

A series of new mannich base derivatives of isoliquiritigenin, liquiritigenin, isolated from *G. glabra* were synthesized, assessed against chloroquine sensitive NF-54 strain of *Plasmodium falciparum*. The most potent analogue in the series was ring cyclised derivative of ISL ($IC_{50}$= 0.065µg/ml). Among mannich base derivatives of liquiritigenin, the most active derivative showed $IC_{50}$= 0.080µg/ml (LTG $IC_{50}$= 4 µg/ml).

We earlier reported antidiabetic, antibacterial, anti-TB, anticancer activity of ISL, LTG. This is the first report of antimalarial activity of ISL, LTG, its derivatives. Hence the natural products can give good lead in the area of drug discovery.



ISL derivative



LTG derivative

**O-4**

# Fe-SPINEL DOPED Naf/DMAP-GO: NANOCOMPOSITE FOR MOLECULAR RECOGNITION

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Nanomaterials are designed materials at the nanometer level to take advantage of their small size and novel properties in applications of sensing, catalysis etc. Graphene oxide seems to be a class of graphene derivatives, possess several oxygen containing groups on its surface, synthesized via chemical exfoliation of pristine $sp^2$ hybridized, 2-D graphene. Although availability of numerous oxygen containing species, it offers a strong hydrophillic nature, sp3 hybrid carbons provide it poor electrical conductivity. Therefore, major attention is on the development of doped or functionalized graphene oxide nowadays in advance material science. Functionalization of graphene oxide with electron rich aromatic compounds, metal or metal oxide nanoparticles, conducting polymer etc is in interest. In continuation of our program of research in the field of material science [1,2], we synthesized a nanocomposite material by doping Fe-spinel ($Fe_3O_4$) on Naf/DMAP functionalized GO [2]. The proposed material was characterized through scanning electron microscopy, transmission electron microscopy, fourier transform infra red spectroscopy, UV Visible, X Ray diffraction and Cyclic voltammetry. The prepared nanocomposite material was utilized for the detection of electrocatalytic reduction of hydrogen peroxide.

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**O-5**

# Design, synthesis and anti-tubercular activity of novel tetrahydroquinoline based hydrazides

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Tuberculosis (TB) predominantly caused by *Mycobacterium tuberculosis* (Mtb) is one of the leading human infectious disease. According to WHO global tuberculosis report, around 9.6 million people fell ill due to TB related complications in 2014, and in the same year around 1.5 million people died due to TB [1]. Although, current anti-TB therapy is effective against non drug resistant Mtb, but multi drug-resistant (MDR) TB has become increasingly prevalent now a days. Recently, emerging cases of extremely drug-resistant (XDR), totally drug-resistant (TDR) forms of TB and its co-infection with HIV have lead to an increasing occurrence of treatment failure [2, 3]. So, to circumvent these problems there is compiling need for the search of novel drugs active against both sensitive and drug resistant strains of Mtb.

In the present study, fifteen novel tetrahydroquinoline based hydrazides were designed, synthesized, characterized using spectral techniques (FTIR, $^{1}$H NMR, Mass and elemental analysis) and *in-vitro* evaluated against *M. tuberculosis* (H37Ra strain) [4]. Synthesized compounds were also evaluated for cytotoxicity against human lung fibroblast cells [5]. Among the titled compounds, two compounds **7g** and **7o** exhibited significant anti-tubercular activity with MIC values below 20 µg/mL, with safety index greater than 9.94 and 10.57, respectively. Structure Activity Relationship (SAR) studies were performed in order to explore the effect of substitution on the anti-tubercular activity of the tested compounds.

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**O-6**

# PROTECTIVE POTENTIAL OF *AVERRHOA BILIMBI* LEAF EXTRACT ON ALCOHOL AND ACETAMINOPHEN INDUCED HEPATOTOXICITY

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**Abstract:** *Averrhoa bilimbi* (*Oxalidaceae)* is one of the most legendary and sacred trees of India. Fruits, leaves are generally used for therapeutic purposes. *Averrhoa bilimbi* has been widely reported for its multiple pharmacological properties such as anti-inflammatory, antioxidant, anti-scorbutic, astringent, anti-bacterial, antimicrobial, anti-atherogenic, antihyperlipidemic and postpartum protective properties. The present study was undertaken to investigate the hepatoprotective activity of ethanolic extract of *Averrhoa bilimbi* leaves against alcohol and acetaminophen induced Hepatotoxicity in albino rats.

Preliminary phytochemicals screening of *Averrhoa bilimbi* leaves extract indicated the presence of sterols, flavonoids, tannins, glycosides and triterpinoids. Acute toxicity study of ethanolic extract of leaves of *Averrhoa bilimbi* was carried out and extracts were found to be safe up to 2000 mg/kg body weight. Hepatoprotective activity were carried out by alcohol induced and paracetamol induced model in rats. Administration of alcohol and acetaminophen to rats caused significant liver damage, as evidenced by the altered serum biochemical parameters. Pretreatment of rats with ethanolic extract of *Averrhoa bilimbi* exhibited marked protection against alcohol and acetaminophen induced hepatotoxicity in comparison with standard drug silymarin.

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O-7

# Density Functional Theory based Investigation of Structure and Conformational Equilibrium Of Oxacalix[4]arene

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**Abstract:** Oxacalixarenes, the functionalised calixarene based supramolecular architectures allow to act as ideal host and recognition vehicles due to preorganised cavity and greater specificity-reactivity of the oxygen centre. Conformational preferences in such architectures determine the fate of applications ranging from membranes, to neurotransmission, to specific drug-receptor interactions, to enzyme catalysis via integration of the structure-function relationship. Hence, knowledge of conformational behaviour is ideal for implementing and designing the oxacalixarenes for further applications. With this endeavour, assessment of conformational equilibrium was explored in gaseous as well as solvation phase using the most recent GrimmeDFT-D3BJ scheme. The role of dispersion forces and non-bonding interaction was also addressed. Furthermore, factors governing the thermodynamic stability, fate of complexation and distribution of electrostatic potential with population analysis (NBO and mulliken); crucial for the analyte recognition were also discussed.

**Keywords:** conformation, DFT, solvation, calix[4]arene, dispersion

**O-8**

## Stim1 inhibitor ML9 promotesdeath signals in cultured ratcardiomyocytes

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ML9 (1-(5-chloronaphthalenesulfonyl)homopiperazine hydrochloride)) is a well-known chemical inhibitor for STIM1-plasma membrane interactions that eventually prevents store-operated $Ca^{2+}$ entry. Furthermore a basal autophagy is protective for cardiac cell survival. However the possible autophagy-mediated cardiomyocyte death have been recently described. But, no reportis available to explain how ML9 mediated autophagy contributes to cardiomyocyte death. To investigate this, Cultured rat cardiomyocytes were incubated with DMEM/M199 media containing 2% FBS for 4 h. To assess the autophagy flux, bafilomycin A1 was used and LC3 processing was determined by Western blot. Cleaved caspase-3 (apoptotic marker)was detected by Western blot. Extracellular lactate dehydrogenase and ROS production were measured following the standard protocols. Cell viability was assessed by Trypan blue exclusion test. Results showed that after 4 h of ML9 treatment, LC3-I as well as total LC3 levels decreased significantlyas compared to the basal levels. These changes persisted even when autophagic flux was blocked using bafilomycin A. No change in beclin-1 protein levels was observed. Incubation with ML9 for 4 h inhibited basal autophagic flux. Moreover, ML9 treatment decreased STIM1 protein levels in the presence or absence of bafilomycin A. Treatments with ML9 resultedon the activation of caspase 3, indication of occurrence of apoptosis. Extracellular lactate dehydrogenase level, nuclear fragmentation and ROS production are also in support of cell death. These data suggest that ML9 inhibited autophagic flux, decreased STIM1 protein leveland induced cardiomyocyte death.

Work supported by FONDAP 15130011, FONDECYT 3150545

**O-9**

# A Novel Sulpha Lipid as Human Topoisomerase I & II inhibitor: Isolation and its Cytotoxicity Screening

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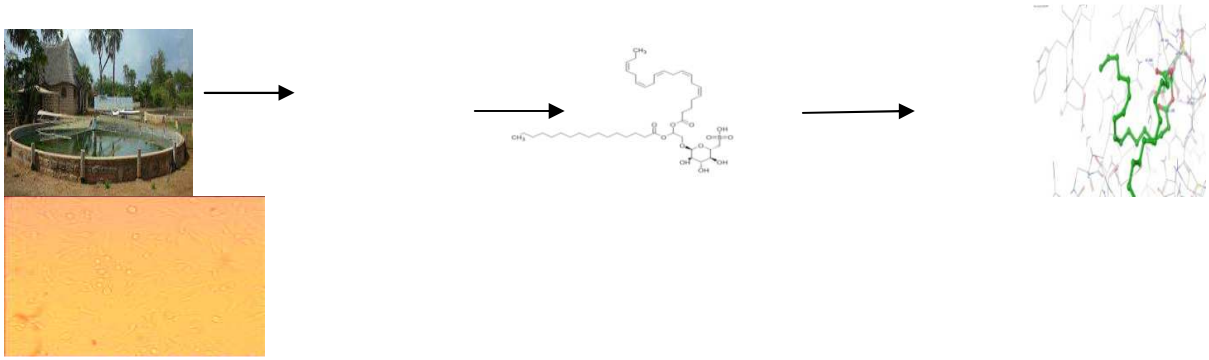
A blue green marine algae *Spirulina platensis* contains an important sulpha lipid Sulpho Quinovosyl Diacyl Glycerol (SQDG). It has been isolated by flash chromatography which is a novel and economical method and characterized by using LCMS (ESI-MS). The isolated compound (SQDG) has been subjected to cytotoxic study by Sulphorhodamine B method on MCF-7 cell lines. The results indicated that SQDG has significant *in vitro* anticancer activity on MCF-7 cell lines with $CTC_{50}$ value of 0.46 µm when compared to the standard quercetin. The isolated sulphalipid bas been docked into the crystal structure of topoisomerase I (1K4T, 3AL2) and topoisomerase II (1ZXN, 3QX3) using Schrödinger suite, 2014-3. The *in silic*o results showed that SQDG is a potent Human topo isomerase I & II inhibitor. Hence the current molecule may act as a lead molecule in anticancer therapy.



**Keywords:** Sulpho quinovosyl diacyl glycerol, Flash chromatography, Topoisomerase 1 & II Poison, MCF-7 Cell lines, cytotoxicity

**O-10**

# β-LACTAM RING: SYNTHESIS AND ROLE IN DRUG DISCOVERY

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β-Lactams have occupied a central role in the fight against bacterial infections over the past several decades. However, bacterial resistance to β-lactam antibiotics by producing β-lactamase is a serious concern and co-administration of a suicide inhibitor of the enzyme restores the activity of these antibiotics. This is done by selectively inactivating β-lactamase due to easy opening of the strained β-lactam ring of suicide inhibitors [1]. From chemical point of view, β-lactams are used as synthons for further functionalization, and are considered as one of the most important aza-heterocyclic frameworks in organic chemistry [2]. Due to their chemical and biological importance, synthesis and properties of *β*-lactam derivatives with various functional groups are important and maintain a rarefied place in the history of organic reactions and pharmaceutical fields.

In continuation of our program of research to develop novel synthetic routes to heterocycles [3], we have reported useful synthetic protocols for constructing β-lactam ring including multi-component reactions and Staudinger reaction [4-6]. We have synthesized highly strained β-lactam ring [4], which is suitable for co-administration as suicide inhibitor of β-lactamase to restore its activity for functioning as efficient antibiotic. Furthermore, we have recently reported the green synthesis of β-lactam ring using a completely new route via carbohydrate activation as one carbon aldehyde equivalent and masked acids as two carbon acetyl equivalent for construction of β-lactam ring [5]. Very recently, we have reported a modified Staudinger protocol for β-lactam synthesis via carbocation catalyzed acetic acid activation [6]. The reported methods for synthesis of β-lactam ring are good alternative to cater the need for academia and industries.

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**O-11**

# Exploration of Interaction Zones of β-tubulin Colchicine Binding Domainof Helminths and Binding Mechanism of Anthelmintics

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**Abstract:** The emergence of anthelmintics resistance due to evolutionary adaptation of helminthes intensifies a pressing need for the development of effective drug. Numerous studies associated with the susceptibility and resistance of anthelmintics to mutations present in the colchicine binding site of β-tubulin and postulated the possible modes of action and its underlying resistance mechanisms. Originally explored for anticancer therapeutics, structural studies of β-tubulin showed that several co-crystal anthelmintic with diverse configurations bind dissimilarly in the colchicine binding site and overlap partially in their binding positions indicating the alternate sites in the colchicine binding domain to modulate tubulin function. The affirmation of such binding mechanisms in helminthes by experimental studies strengthened the binding hypothesis of contiguous sites of preexisting colchicine binding site. First time, we report the three interaction zones (zones vide -1 to -3) of this domain and developed structure-based pharmacophore models coupled with molecular docking technique to unveil the binding hypotheses. Zone wise structure-based pharmacophore models of anthelmintics interacting inβ-tubulin 'colchicine domain' were built using the dock poses predicted with *H. contortus* β-tubulin homology model and the resultant hypotheses were mapped among the finitely perturbed dock states of anthelmintics. Structure-based hypotheses were refined to essential three point pharmacophore features that captured recurring and crucial non-covalent contacts with receptor and concluded three characteristics necessary for optimal binding: a conserved pair of H bond acceptor (HBA) that formed H bond with Asn226 residue and an aliphatic moiety of molecule separated by 3.75 ± 0.44 Å. Further, an aliphatic group or a heterocycle (third component) disjoined by a distance of 11.75 ± 1.14 Å with respect to conserved aliphatic site formed the frame for zone-2 specific anthelminthic. Alternatively, an additional HBA can be organized in place of third component to establish H bonding with Asn204. We foresee that zone-2 anthelmintics with high affinity can be designed effectively by close adaptation of pharmacophore feature patterns and its geometrical constraints.

**Keywords:** Anthelmintics, β-tubulin, colchicine, structure-based model, pharmacophore, docking

**O-12**

# *INVITRO* HYPOGLYCEMIC POTENTIAL OF SELECTED DIHYDROXY FLAVONES

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**Objective**: The objective of the present study is to screen the effects of selected substituted dihydroxyflavone for its *invitro* antidiabetic effect by finding the potential to inhibit the enzymes α-Glucosidase.

**Materials and Methods**: The dihydroxy flavones used in the present study includes 2',3'- dihydroxy flavone (DHF) and 2', 4' dihrdroxy flavones(DHF). They were synthesized using standard procedures. *In vitro* α-glucosidase inhibitory activity was evaluated by Li et al., 2004. α-Glucosidase inhibitory assay is based on the breakdown of maltose to glucose. 200 µl of α -glucosidase solution was pre-incubated with the test and control samples for 5 min. The reaction was started by adding 200 µl of sucrose and it was terminated after 30 min incubation at $37^0$C by heating at 90–$100^0$C. The liberated glucose was determined. The different concentration of the flavonoid ( 0.1, 0.3, 1, 3,10, 30, 100, 300, 1000 (µM/ml) were used and the experiment was done for triplicate sample. The standard antidiabetic drug used in the study was Acarbose.

**Results**: The selected Dihydroxy flavones 2',3'- DHF and 2', 4' DHF showed significant invitro anti diabetic activity when compared with standard drug acarbose. The IC50 value of 2',3'- DHF and 2', 4' DHF was found to be 0.47µM/ml, 46.37 µM/ml respectively.

**Conclusion**: The study reveal that 2', 3' DHF have excellent invitro antidiabetic effect in α-Glucosidase inhibitory assay model.

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| S.no | Concentration (µM/ml) | %Inhibition of α - glucosidase | | |
|---|---|---|---|---|
| | | 2',3'- dihydroxy flavone | 2',4'- dihydroxy flavone | Acarbose |
| 1 | 0.1 | 33.81±0.33 | 12.74±0.11 | 11.34 ±0.35 |
| 2 | 0.3 | 41.51±0.67 | 16.04±0.22 | 18.87±0.57 |
| 3 | 1 | 51.26±0.67 | 25.47±0.67 | 35.29±0.61 |
| 4 | 3 | 56.29±0.22 | 35.38±0.56 | 38.86±0.08 |
| 5 | 10 | 67.61±0.00 | 44.18±0.56 | 45.41±0.34 |
| 6 | 30 | 71.23±1.00 | 49.06±0.22 | 48.70±0.79 |
| 7 | 100 | 79.87±0.22 | 59.28±0.78 | 54.87±0.06 |
| 8 | 300 | 86.48±0.89 | 67.61±0.22 | 70.67±0.06 |
| 9 | 1000 | 89.31±1.11 | 88.36±0.67 | 97.29±0.12 |
| | **$IC_{50}$** | **0.47µM/ml** | **46.37 µM/ml** | **23.84µM/ml** |

**O-13**

# Artificial Neural Network Model to Recognize Potential MAO-B inhibitors for Parkinson's Treatment

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Parkinson's disease is an incurable, chronic progressive condition involving dysfunction of dopamine producing neurons in the brain. The pathologically the disease is characterized by degeneration of dopaminergic neurons in the substantianigra pars compacta and the presence of Lewy bodies, cytoplasmic aggregations of the protein α-synuclein in brain neurons. Parkinson's is the 2nd most common neurodegenerative disorder after Alzheimer's and affects about 0.3% of general population world-wide and is estimated to occur in about 1% in individuals aged 60 years.

L-DOPA a precursor to a class of neurotransmitters called catecholamine including – dopamine, is the mainstay of Parkinson's disease therapy. Toimprove treatment efficacy and decrease motor complications, levodopa may be augmented with a dopamine agonist or MAO-B inhibitors. The primary rationale for using selective MAO-B inhibition in Parkinson's disease is that it enhances striatal dopaminergic activity by inhibiting the metabolism of dopamine, thereby improving Parkinson's disease motor symptoms. To some extent theoretical, rationale for the use of selective MAO-B inhibitors in patients with Parkinson's disease is that they may modify disease activity or be neuroprotective.

Lazabemideand Safinamideweretwo reversible and selective inhibitors of monoamine oxidase B (MAO-B) that were under development as an antiparkinsonian agent. Common adverse events in clinical trials were nausea, dizziness, tiredness, headache and backache. The molecules were never marketed due to their adverse effects.

The pharmacophore representation of Lazabemide and Safinamide were generated using vROCS and the pharmacophores were screened against ZINC small molecule database consisting of 50000 compounds. The Screening identified 500 compounds most similar to Safinamide and Lazabemideeach. Out of these 500 compounds 4 compounds namely: 2-[1-(4-ethoxyphenyl)ethylamino]ethanol,4-Isopropoxy-benzylamine,4-Ethoxy-benzylamine,-o-Tolyloxy-benzylamine, were found to commonly similar to both Safinamide and Lazabemidehe similarity on basis of Tanimoto coefficient. A common scaffold of 4-ethoxyphenyl methanamine was found to be present all the four aforementioned compounds. Based on the scaffold a combinatorial library was built by adding suitable linker's and building blocksusing SMILIB 2.0.A total of 60 novel compounds were generated out of which only 46 followed the Lipinski's rule of 5.These 46 compounds were chosen as potential lead molecules as MAO B inhibitors for treatment of Parkinson's Disease.

Simultaneously a Neural Network model was built to facilitate classification of small molecules as MAO B inhibitors or not. For this purpose a library of 230 MAO B inhibitors was built on basis of already available literature, another 204 compounds were chosen at random from Pubchem database to be utilized as control. Literature was comprehensively analyzedto make sure that none of the 204 compounds have MAO B inhibitory activity.
Web CDK 2.0 was employed to generate descriptors for each of the 434 compounds (230 MAO B inhibitors + 204 control compounds).A classification variable called GROUP was introduced in the spreadsheet. MAO B inhibitors are categorized as 1 and controls as 0.Linear Regression was performed to achieve feature selection so that only the most important variables to classify MAO B inhibitors. xlogp, toposhape, bpol, SP7, SP3, SP0, SP1 were recognized to be important based on p values.Multilayer perceptron neural network based model was developed by taking the

aforementioned properties. The gene expression raw data of each sample was taken as covariates (input layers) and "grouping" as the dependent variable. All data were standardized, 67.8% of data was allocated as training set and the remaining 32.2% as test set. Neural network thus built, was found to be capable of classifying MAO B cases (1) as cases with >90.8% accuracy and controls (0) as controls with 100% of accuracy. The overall accuracy of the MLP network was an impressive- 95.6%.

The 47 molecules from the combinatorial library were screened using the Neural Network Model built. 19 molecules were recognized as potential MAO-B inhibitors. These 19 molecules were subjected to Virtual Screening against the crystal structure of MAO-B (PDB ID: 1GOS) with molegro virtual docker and (2S)-2-[({[4-(methoxymethyl)benzyl]amino}oxy)amino]propanoic acid was found to have the best binding affinity against MAO-B with a molegro score of - 68.57 with 13 hydrogen bonds. This molecule can be further studied to be developed a potential antiparkinsonian lead molecule.

**O-14**

# Regioselective *ortho*-Halogenation of Aryl C-H bonds

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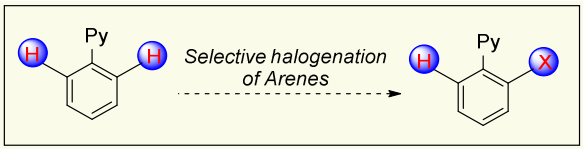
The development of mild methods for the selective functionalization of carbon-hydrogen bonds to C–X (heteroatom) bonds remains a significant challenge in organic synthesis [1].Transition-metal-catalysed C-H bond functionalisation *via* directing group assisted C-H bond activation has witnessed substantial progress during the past decades [2]. General methods for the construction of these building blocks are electrophilic halogenation, *ortho*-metalation followed by halogen quenching have commonly involved multiple steps, toxic reagents, multiple regioisomeric products and harsh reaction conditions [3]. We have developed a concise, versatile and practical method for the *ortho*-chlorination, *ortho*-bromination and *ortho*-iodination of aryl compounds. The significant advantage of this transformation is the creation of the carbon-halogen bond by use of readily available and cheap halide salts as formal nucleophilic halogenating reagents under mild reaction conditions.




**Scheme 1.** DG-assisted transition-metal-catalysed regioselective *ortho* $C_{Ar}$–H halogenations of arenes.

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**O-15**

# Design and development of flavonoid derivatives as androgen receptor antagonists

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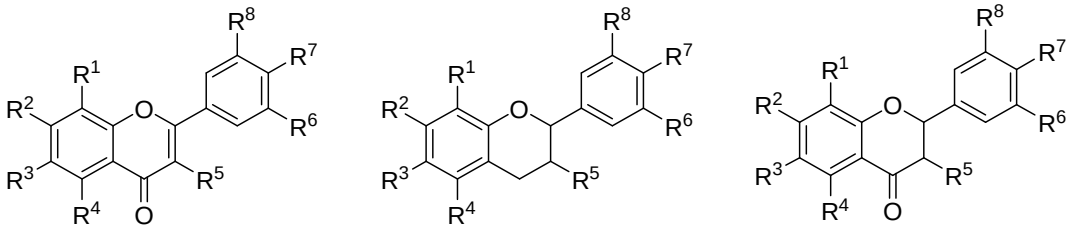
**Abstract:** Prostate Cancer (PCa) is one of the most frequently diagnosed noncutaneous tumors worldwide.[1] Drug discovery from plant-based compounds has since long been a paradigm for the treatment of various diseases. In this journey, a large number of plant-based products have taken a lead position in the market as active pharmaceutical agents.2-phenyl-4H-chromen-4-one, 3,4-dihydro-2-phenyl-2H-chromene and 2,3-dihydro-2-phenylchromen-4-one derivatives are highly useful synthetic intermediates have found numerous applications in the area of therapeutics.[2, 3] The flavonoid analogs were designed by the structural modifications (Fig. 1).




2-phenyl-4*H*-chromen-4-one  3,4-dihydro-2-phenyl-2*H*-chromene  2,3-dihydro-2-phenylchromen-4-one

Fig. 1 Structural modifications of the three potent structure of AR antagonist

In a previous study, we have reported the design and synthesis of several oxobenzimidazoles and thiazolidinediones that demonstrated the relevant cytotoxicity and pharmacokinetic properties.[4] Encouraged by previous studies and in continuation of our effects, co-crystallized ligand-protein structures have been used effectively to both understand the functional mechanisms of the receptor and for structure-based drug design (Fig. 2).

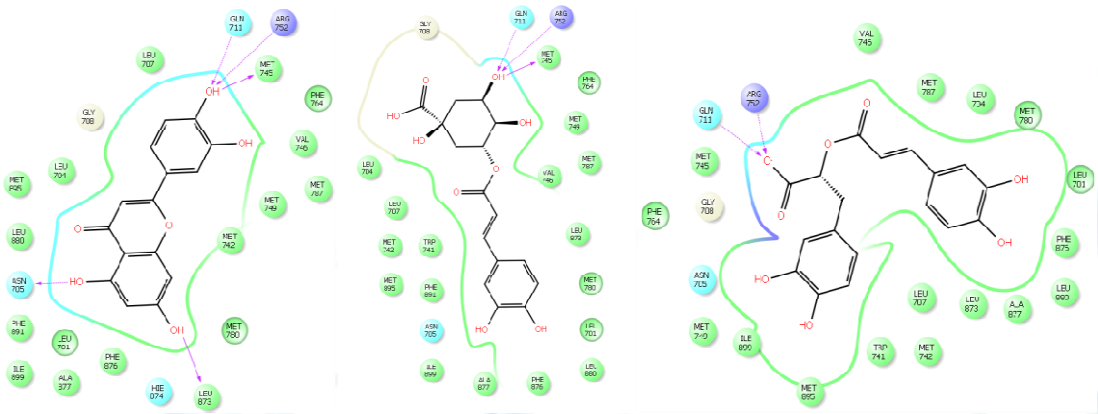


Fig. 2 Predicted binding mode of the active compounds in the AR crystal structure

We have successfully synthesized a series of flavon-3-ols, flavone and flav-3-ene derivatives with various substitution groups aiming at the discovery of potential AR antagonists. *In vitro* antioxidant and anti-prostate cancer activities of the flavonoid derivatives were evaluated. In addition, DFT calculations were clearly confirmed the stable conformer of the compound. All the compounds

showed compliance with the standard range of known drugs ADME properties. We, further, intend to investigate the target site and to study the *in vivo* anticancer activity of the active compounds.

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**O-16**

# Modulation of Strength and Sorption Capacity of Carboxymethylcellulose Hydrogels in Presence of Ester Bonded Gemini Surfactants

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The Carboxymethylcellulose-surfactant hybrid hydrogels were prepared using carboxymethylcellulose sodium salt and Gemini surfactants in urea solution. The structure and morphology of the synthesised hybrid hydrogels were characterised using FT-IR spectroscopy and scanning electron microscopy, respectively. The selling behaviour of synthesized hybrid hydrogels were investigated in distilled water in presence of different salts and differing pH's. The swelling capacity of these hydrogels were found to decrease with an increase in the charge of the metal cation ions ($Al^{3+} < Ca^{2+} < Na^{+}$). The Rheometeric observations reveal an increase in the elastic modulus (G) of the CMC hydrogel on addition of surfactant, indicating an increase in the mechanical strength of the CMC hydrogel, on addition of Gemini surfactant. However, at higher concentrations surfactants the G values progressively decreased. The effect of added surfactants on gelation temperature of CMC was investigated through oscillating temperature sweep. The gelation temperature of CMC-urea + 16-E2-16 surfactant was found to be higher than that of CMC-urea + 14-E2-14 Gemini surfactant. The encapsulation capacity of synthesized CMC-urea surfactant hybrid hydrogel systems were explored for sorption capacity of various hazardous polynuclear aromatic hydrocarbons (PAHs) from their aqueous solutions. The observed results suggest that sorption of PAHs using CMC-urea + surfactant hydrogel systems can be a valuable approach towards safer remediation of groundwater contaminated by toxic organic compounds.

**O-17**

# Discovery of antimicrobial peptides from proteome dataset using a novel *insilico* Cluster approach

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In the midst of discovery of novel drugs against multidrug resistant pathogens, antimicrobial peptides (AMPs) are under focus for its broad spectrum activity. AMPs are indivisiblepart of the innate immune system especially in invertebrates, performing a wide range ofbiological activities, mainly immunomodulatory andantimicrobial activity against variouspathogens. The unique feature of AMPs is their specific mode of action against bacterial cells, thus considered as a potent alternate for conventional antibiotics. Considering these facts, the scientific community is in search of potential AMPs from different sources including invertebrates. In this study, a novel *in silico*cluster approach has been framed to discover short antimicrobial peptidesequences from the proteome library of freshwater prawn, *Macrobrachium rosenbergii*and the efficiency of the identified peptides were demonstrated against various bacterial pathogens. Out of 19,915 sequences present in the prawntranscriptome, 660 short sequenceswith putative antimicrobial activity were scrutinized usinga series of *in silico*analysis based on the antimicrobial propensity of each amino acid and their order of arrangement. Further, the scrutinized sequences were analysed for the hydrophobic and amphipathic property to screen peptides with better membrane binding/disruption activity which finally resulted in five AMPs with an average length of 15 residues. Interestingly, all the identified peptides exhibited bactericidal activity against a wide range of pathogens and preliminary mechanistic analysis revealed that all the peptides disrupted the membranes of the bacterial pathogens. Thus, it is possible to conclude that the described cluster approach could be efficiently used to discover antimicrobial peptides from the proteome database. Moreover, further customization of the parameters in this approach would bring out many more antimicrobial peptides from nature which may serve as better therapeutic agents against various pathogenic infections.

**O-18**

# Silver-Catalyzed Denitrative Sulfonylation of Nitrostyrenes: A Convenient Approach to (*E*)-Vinyl Sulfones

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Vinyl sulfones constitute an important class of compounds with diversified biological activities and synthetic applications.[1–5]. Substituted vinyl sulfones have received overwhelming attention in medicinal chemistry and the pharmaceutical industry owing to their wide scope of utilization as cysteine protease inhibitors,[6] antibiotic TAN-1085,[7] and HIV-1 integrase.[8]

Very recently, decarboxylative sulfonylation reactions of cinnamic acids[9] were reported, and this led us to hypothesize that denitrative sulfonylation reactions of nitrostyrenes, readily available by the Henry reaction, could be a convenient way to access vinyl sulfones. In several instances, nitrostyrenes have been used for denitrative C–C bond formation by an addi- tion/elimination reaction.[10] Considering the above points and our continued work on the functionalization of alkenes,[11] we report herein a convenient catalytic approach to (*E*)-vinyl sulfones from nitrostyrenes and sodiumsulfinates.

The first utilization of nitrostyrenes (readily available by the Henry reaction) for a highly stereoselective, convenient, and catalytic synthesis of (*E*)-vinyl sulfones at room temperature was investigated. The protocol involves efficient silver-catalyzed denitrative radical cross-coupling of nitrostyrenes and sodium sulfinates by using potassium persulfate as an additive to complete the catalytic cycle.

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**O-19**

# Modulation of Glut4 during adipogenesis in 3T3L1 correlates with expression of LXR alpha

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Adipogenesis is a complex biological process involving synchronised interplay of different nuclear receptors. Aberration in the process leads to obesity and associated disorders [1,2]. In the present study we tried to investigate the change in gene and protein expression of major adipogenic proteins in response to PPAR gamma activation. It has been reported earlier that glucose transporter-4 (Glut4) undergoes down regulation during the initial phase of adipogenesis due to binding of trans-acting factors in Domain I [3]. We tried to elucidate the correlation between LXR alpha and Glut4 through activation of PPAR gamma with rosiglitazone, FMOC-L-leucine and GW9661. FMOC-L-leucine enhanced Glut4 expression much earlier in the adipogenic process and was associated with enhanced LXR alpha expression. Moreover, the translocation of Glut4 from nuclear region to cytoplasm and inner membrane side was associated with high degree of co-localization with LXR alpha protein. Immuno-precipitation of PPAR gamma and LXR alpha during different stages of adipocyte differentiation with and without FMOC-L-leucine was done and analysed using LC-MS/MS. From the results, it can be pointed out that LXR-alpha, a glucose sensing protein, is responsible for the enhanced expression of Glut4 in adipocyte differentiation process.

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**O-20**

# Various Spectral Methods for the Characterization of Alpha-amylase Inhibitors from the Roots of *Stereospermum colais*

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Diabetes, a metabolic disorder characterized by hyperglycaemia, occurs due to defects in insulin secretion/ insulin action and affects various organs [1]. Inhibition of α-amylase involved in carbohydrate metabolism is considered as one of the most important therapeutic approach for controlling post-prandial hyperglycaemia by diminishing the absorption of glucose metabolised from starch. Natural products isolated from various higher plants have been providing novel, clinically active antidiabetic drugs. This report aims to provide a scientific basis to the traditional knowledge on medicinal plants and specifically deals with the phytochemical investigation on the roots of *Stereospermum colais* (Family: Bignoniaceae). Column chromatographic fractionation of acetone extract using varying polarities of hexane-ethyl acetate solvent system yielded 7 compounds viz, β-sitosterol, 2-(4′-hydroxyphenyl) ethyl undecanoate, 2-(4′-hydroxyphenyl) ethyl pentadecanoate, 5α-ergostan-7, 22-dien-3β-ol, ursolic acid, lapachol and pinoresinol. The structure of the compounds were characterized by various spectral methods like UV, IR, NMR, HRMS etc. All compounds were isolated for the first time from the species and screened for its α-amylase inhibition potential [2]. Ursolic acid, lapachol and pinoresinol showed significant inhibition potential compared to acarbose, a standard α-amylase inhibitor.

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**O-21**

# Design and Synthesis of Hit Molecules Bearing Novel Pteridine Scaffold as Dual Aurora-B and CDK2 Kinase Inhibitors as Apoptosis Inducer

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**Abstract:** Cellular proliferation is govern by different cell cycle stages. It has been proved that 90% of human cancers are due to abnormality in cell signalling pathways. A related kinase family members, Cyclin Dependent Kinase (CDK) and Aurora Kinase (AurK), are interesting targets for potential dual kinase inhibitors drug development approach [1]. Various molecular modelling approaches like 3D-QSAR [2] and molecular docking were used for designing of novel molecules bearing pteridine scaffold [3]. All synthesize molecules were screened for *in-vitro* cytotoxicity study on 7 different cancer cell lines [4] and they showed $IC_{50}$ in range of 0.2 µM to 100 µM. *In-vitro* enzymatic inhibition was evaluated on AurK and CDK-2 with % inhibition and $IC_{50}$ of all compounds in µM range [5]. Based upon results of these two studies, eight most potent inhibitors were evaluate by Colony forming assay. Best molecules were further estimated in cell signalling inhibition using cell cycle analysis (PI staining) and found G2/M arrest in cancer cells. Apoptosis assay was also performed using Annexin-V FITC staining and 2 potent molecules produced early apoptosis in low µM range. Both studies were performed on sophisticated MUSE® analyser. These molecules were screened for *in-vivo* animal models. Preliminary, molecules were checked in p388/D1 murine luekamia model for increment of life span study. 2 Molecules were found active with increase lifespan of >60% as compared to disease control group [6]. Further, these molecules were evaluated in early stage subcutaneous animal model [7] where cancer cells injected in the Balb/C mice and found > 60% tumor growth inhibition by both molecules as compared to disease control group. Serological parameters were also evaluated. Histopathological examination also supported decrease in tumorigenic condition with slow tumor growth in treatment group. In summary, we have found hit molecules which could be developed further with better pharmacological activity and improved pharmacokinetic efficacy in future.

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**O-22**

# Coaxial electrospray fabrication of paclitaxel loaded solid lipid microparticles for cancer targeting

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**Abstract:** Cancer is one of the major cause of mortality in the patients being diagnosed with it, in spite of several chemotherapy and other available treatments. Drug efflux-transporters serve as a major barrier to anticancer drugs at the target site. One strategy to enhance the therapeutic efficacy of drugs against cancer is to increase their available concentrations at the desired site (Ho et al., 2007, Taylor et al., 1997). Paclitaxel (PTX)-loaded solid lipid microparticles (SLM) are prepared by Coaxial Electrospray method with high encapsulation efficiency. Biocompatible and biodegradable stearic acid is used to produce the solid matrix. Drug stability, as assessed by encapsulation efficiency (EE; %), particle size, and polydispersity index (PDI), are examined with in vitro release of PTX from SLM. PTX-SLM are characterize for their size measured by Zetasizer Nano-ZS, Malvern, UK and by scanning electron microscopy (SEM) which are of less than 2 µm size. The maximum percentage entrapment efficiency (%EE) determine using ultra-performance liquid chromatography (UPLC). The release pattern of PTX from PTX-SLM reveals sustain release manner of PTX, which is desirable. The percentage cytotoxicity of blank SLM are within the acceptable range. Cytotoxicity assay reveals that encapsulation in microparticles did not compromise the antitumor efficacy of PTX against SKOV-3 ovarian cancer cells. Pharmacokinetic study results are supposed to enhance the bioavailability of PTX in rats for SLM in comparison with Taxol.

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**O-23**

# The Discovery of Novel Enoyl-acyl Carrier Protein Reductase Inhibitors: A Multiple Complex Based Pharmacophore Modelling Approach

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Enormous efforts have been made in the past to develop inhibitors against the potential therapeutic target, Enoyl-acyl Carrier Protein Reductase from *Mycobacterium tuberculosis (Mt*InhA), to combat resistance.[1-6] Over a dozen of small molecules have been crystallized to characterize the structural basis of inhibition. However, the pharmacophoric studies accomplished so far have not incorporated and evaluated all the interactions patterns of these complexes simultaneously. Therefore, an attempt was made in this direction to identify the unique pharmacophoric features that can be employed to prioritize the molecules against *Mt*InhA. With efforts on rigorous validation and expertise, we have identified such complimentary features from natural compounds that that can be used as initial hits. We look forward to experimentally validate the computational hypotheses in order to test the inhibitory roles and understand the biological profile of these compounds.

**Key-words:** pharmacophore models; receiver-operator characteristic; Güner-Henry score; enrichment study

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**O-24**

# Isolation, characterization and biological activity of a new ursane-triterpene from *Phlebophyllum kunthianum*

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New Drug discovery research holds key position in pharmaceutical industries as pharmaceutical industry has the fundamental that are going to lead to increasing demand for health care. The process of discovery of new drugs is highly tedious and in order to discover a new drug approximately 1500 million US $ and 15-20 years required. Plants have been recognized for many years as a source of new therapeutic agents and of structural diversity as most of the drugs currently in the market either isolated from plants or plant's derivatives. Keeping in view importance of medicinal plants as a source of new therapeutic agents and continuation of our effort to isolate and identify the new leads from medicinal plants [1-3] recently, by pharmacological approach, we have isolated new ursane-triterpene from *Phlebophyllum kunthianum* [4]. The details isolation procedure, structural elucidation and pharmacological activity of the isolated ursane-triterpene will be discussed during presentation.

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**O-25**

# Antimicrobial and antioxidant activities of minor millet extracts

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**Abstract:** *In vitro* antimicrobial assay and antioxidant property of the three genders of minor millets *(Echinochloa crus-galli*, *PanicummiliaceumL*, *Panicumsumatrense*) were evaluated.Extracted phenolic acids and one flavonoid were characterized by various analytical techniques. Antimicrobial assay of six extracts of three species were evaluated against bacterial strains of *Staphylococcus aureus* (MTCC 96), *Bacillus megaterium*(*MTCC-428*), *Escherichia coli* (*MTCC 443*) and *Pseudomonas aeruginos (MTCC1688*) and fungal pathogens *Aspergillus niger*(MTCC 282)and *Fusarium oxysporum (MTCC-1755*). It is concluded from the results that phytochemicals are responsible for such inhibition of multi resistance microorganisms and could be a source of new antibacterial drugs.

$IC_{50}$ for various extracts were determined for DPPH scavenging, bleaching of β- carotene and percentage inhibition of $H_2O_2$ and compared with standard positive controls viz. butylated hydroxytoluene (BHT) for DPPH, propyl gallate for β-carotene and ascorbic acid for $H_2O_2$ assay.

**Various part of *Echinochloa crus-galli*(Barnyard Millet) out of all parts, seeds were used for further investigation**

**Keywords*:*** Antimicrobial assay; Antioxidant activity; Phenolic content; flavonoid

**O-26**

# An efficient and direct synthesis of substituted 2-phenylquinoline-4-carboxamides from 3-substituted-3-hydroxyindolin-2-ones

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**Abstract:** A simple and direct synthesis of substituted 2-phenylquinoline-4-carboxamides from 3-substituted-3-hydroxyindolines in presence of ammonium acetate is described. The developed protocol also allows synthesis of the carboxamidemoeity directly from isatin and acetophenone in one pot under optimized conditions. The protocol has the merits of simple reaction conditions, and good yields of products.

**Keywords:** 2-Phenylquinoline-4-carboxamide, ammonium acetate, 3-hydroxyindolin-2-ones

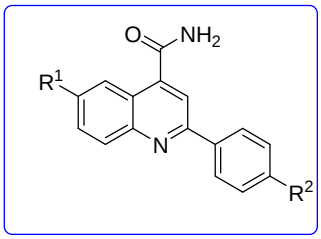
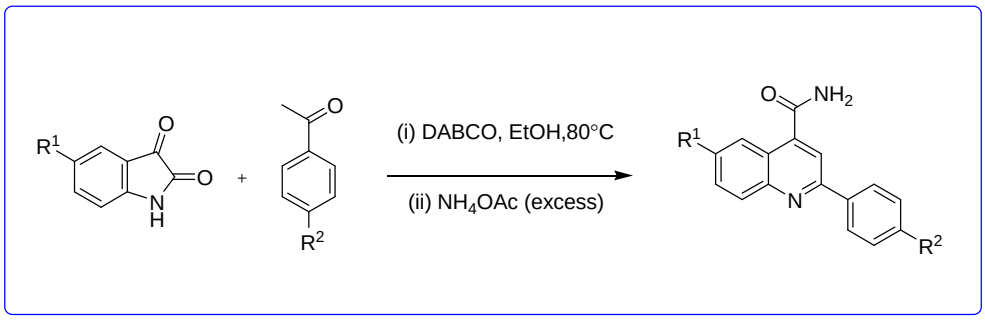



**Figure 1.**Synthesised Compound Substituted 2-arylquinoline-4-carboxamides




**Scheme 1.**One pot synthesis of substituted2-arylquinoline-4-carboxamides

**Reference:**

1. K N Tiwari, D Bora, G Chauhan, D Yadav, K Sharma, A Thakur, L Singh, V Tripathi, Synth.Commun.46, 2016, 620.

**O-27**

# One-pot conversion of Ofloxacin using tetra butyl ammonium bromide and their Biological Activity

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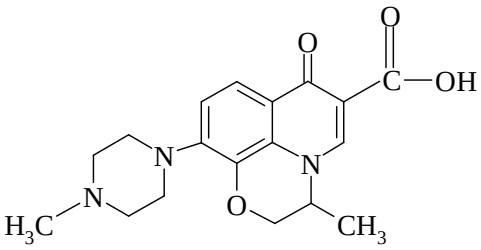
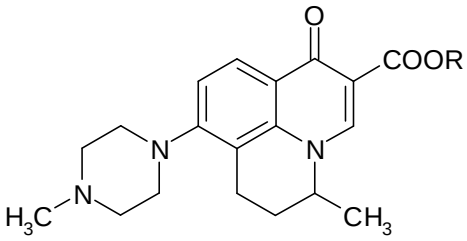
**Abstract**: Substituted-3-methyl-10 (4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H[1,4] oxazino[2,3,4-ij] quinoline-6-carboxylate ring are synthesized under the influence of tetra butyl ammonium bromide catalysis. The method is known to work satisfactorily for optically active acids having epimerisable α-hydrogen. All synthesized derivatives evaluated for their Biologicall activity. The compounds show significant antibacterial activiy against S. aureus (gram (+)ve) and E. coli (gram (–)ve) bacteria when compared with standard drug Ofloxacin and the compound also show significant antifungal activity against A.niger fungi when compared with standard drug Ketoconazole.

***Result and Conclusion:*** Synthesized derivatives evaluated for their Biologicall activity.The compounds show significant antibacterial activiy against S. aureus (gram (+)ve) and E. coli (gram (–)ve) bacteria when compared with standard drug Ofloxacin and the compound also show significant antifungal activity against A.niger fungi when compared with standard drug Ketoconazole.

**Keywords:** Ofloxacin, Phase Transfer Catalyst, Biological Activity

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**O-28**

# Syntheses of Families of Enantiopure and Diastereopure Octahedral Cobalt Catalysts and their utility in Organic Synthesis

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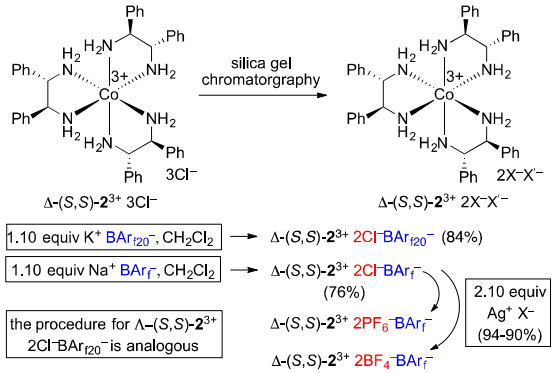
**ABSTRACT:** Diastereomeric salts such as Λ-$[Co((S,S)\text{-dpen})_3]^{3+}$ $3Cl^-$ (Λ-(*S*,*S*)-**1**$^{3+}$ $3Cl^-$) or Δ-(*S*,*S*)-**1**$^{3+}$ $3ClO_4^-$ have been synthesized (60-65%) by the reactions of $CoX_2$ (X = OAc, Cl) or $Co(ClO_4)_2$ with (*S*,*S*)-1,2-diphenylethylenediamine [1]. Anion metatheses lead to large families of lipophilic salts Λ- and Δ-(*S*,*S*)-**1**$^{3+}$ $2X^-X'^-$ (X/X' = Cl/$BAr_f$ ($BAr_f$ = $B(3,5\text{-}C_6H_3(CF_3)_2)_4$), $PF_6$/$BAr_f$, $BF_4$/$BAr_f$, $PhBF_3$/ $BAr_f$, Cl/$BAr_{f20}$ ($BAr_{f20}$ = $B(C_6F_5)_4$), $BAr_f$/$BAr_f$, $BAr_{f20}$/$BAr_{f20}$, $BF_4$/$BF_4$, $PF_6$/$PF_6$) (scheme-1). These have successfully utilized as hydrogen bond donor catalysts [2] for the enantioselective organic synthesis [3].




**Scheme-1:** Synthesis of Werner salts

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**O-29**

# GENOMIC ANALYSIS OF TOLERANT BACTERIA OBTAINED FROM *PARTHENIUM HYSTEROPHORUS* L. AMENDED SOIL

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**ABSTRACT:** *Parthenium hysterophorus* L. is an exotic but nuisance weed of India. Its invasion causes changes in above-ground vegetation and below-ground soil nutrient contents thereby reducing pasture productivity by 90%. To assess the impact of *Parthenium hysterophorus* L., bacterial culture was performed over a period of 45 days using dilution plate method and results obtained were compared with control. Genomic analysis was also done to identify the bacteria of different culture plate. Genomic analysis of bacterial colony (Δ PH-1) having punctiform- entire; shape and margin whose percentage was maximum in control and all the combination of *Parthenium* amended soil was identified as *Aeromonas punctata* strain JM10 (Genbank Accession Number: GU205197.1) and whose length of consensus sequence is 1418bp. Gram staining test showed that it is gram –ve bacteria. *Parthenium* resistant irregular - undulate colony (Δ PH-2 and Δ PH-3) which gradually increased in number during the experiment, was identified as *Bacillus cereus* strain MBL13 (Genbank Accession Number: GQ148914.1) and *Bacillus* sp. BFF-3 (Genbank Accession Number: EF031071.1) and their consensus sequences were 1420bp and 1427bp respectively. On gram staining both ΔPH- 2 and ΔPH-3 were found to be gram +ve. The paper deals with detailed study of all these obtained bacteria.

**KEYWORDS:** *Aeromonas punctata*, *Bacillus*, resistant, gram staining

**O-30**

# Remarkable anticancer activity of ternary copper (II) and oxovanadium(IV) complexes in red light with low dark toxicity

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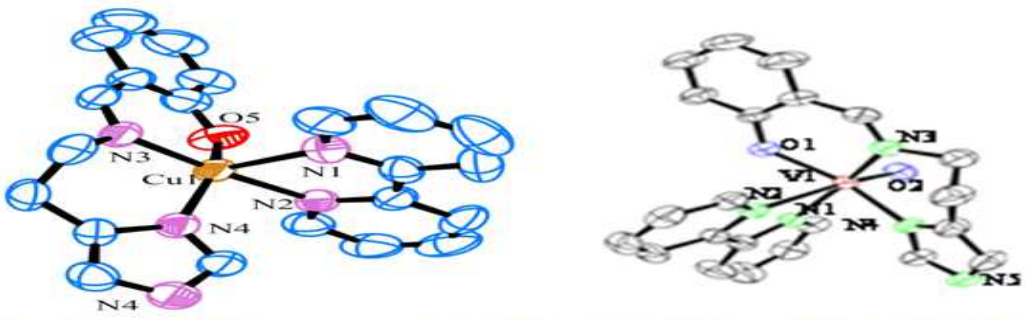
Current growing interest in small molecules that are capable of binding and cleaving nucleic acids under physiological conditions is related to their utility in designing and developing of new drug discovery. By virtue of their tunable coordination geometry, versatile redox potential and diverse reaction mechanism transition metal complexes attracting towards metal-based drug discovery. Copper and vanadium is a bio-essential,biocompatible element and have more biological importance and also have low energy d-d absorption bands which is an essential criterion for Photo Dynamic Therapy. The serendipitous discovery of cisplatin by Rosenberg in the mid 1960s and its introduction to clinic in 1970s, metal based therapeutics entered a new era.

The present work deals with the synthesis, characterization and biological activity of new ternary copper (II) and oxovanadium(IV) complexes of salicylaldehyde-histamine Schiff base ligand and planer polypyridyl bases. Copper (II) complexes of Cu(sal-His)(bpy)]ClO4 [1], Cu(sal-His)( phen)]ClO4 [2], Cu(sal-His)(dppz)]ClO4 [3] and oxovanadium(IV) complexes of [VO(sal-His)(bpy)]ClO4 [4] and [VO(sal-His)(acdppz)]ClO4 [5] were prepared. Various analytical techniques like IR, Mass, UV-vis, conductance are used to characterize the prepared complexes. The biological activities like interactions with double stranded calf thymus DNA and photoinduced DNA cleavage activities were performed. The complex 2-5 showed very good DNA binding affinity which were measured by UV-vis absorption titration method and ethidium bromide displacement assay. The complexes also show nuclease activity in presence of cellular reducing agent glutathione (reduced form). The dppz complex 3 shows very good DNA photocleavage activity in UV-A light of 365 nm as well as red light of 647 nm. The acdppz complex 5 shows the vanadium centered d-d transitions at ~585 nm in the UV region.




Single crystal XRD structures of Cu(sal-His)( phen)]ClO4 and [VO(sal-His)(bpy)]ClO4

**Reference:**

1. Samya Banerjee, Akanksha Dixit, K Sesha Maheswaramma, Basudev Maity, Sanjoy Mukherjee, Arun Kumar, Anjali A Karande, and Akhil R Chakravarty, Photocytotoxic ternary copper (II) complexes of histamine Schiff base and pyriryl ligands, J.Chem. Sci, Vol.128, No.2, February 2016, pp.165-175.
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**O-31**

# Review of chemical approaches on drug development and sustainability (Alchemy to till)

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Medicinal chemistry plays vital role in consecutive drug discovery. Day to day many novel drugs are introducing to cure varioussolemndiseases. It is too difficult to maintain the endowment of ethologic liveliness and may even effect its duration. The medicinal chemist is experiencing significant changes in the last few years to establish sustainableand combinative technologies via greenchemistry. The present discussion gives a gist on how a medicinal chemist to extend the better drug discovery for quality life.The ancient aspect could contribute sagacity in how to develop the present mode byStructural Activity Relationship (SAR) studies and combinatorial techniques in drug discovery with thischemist achieves the creative and innovative role that afford to past success.

**Reference:**

1. Samya Banerjee, Akanksha Dixit, K Sesha Maheswaramma, Basudev Maity, Sanjoy Mukherjee, Arun Kumar, Anjali A Karande, and Akhil R Chakravarty, Photocytotoxic ternary copper (II) complexes of histamine Schiff base and pyriryl ligands, J.Chem. Sci, Vol.128, No.2, February 2016, pp.165-175.
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4. Lindsley, C. W. (2016) Lost in Translation: The death of basic science. ACS Chem. Neurosci. 7, 1024.
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**O-32**

# Synthesis and evaluation of a tag-free photoactive phospho-ceramide analogue-1 (PCERA-1) probe to study immunomodulation in macrophages

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Phospho-ceramide analogue-1 (PCERA-1), is a potent modulator of macrophage activity and inflammation in *vivo*and in *vitro*. We have previously shown that PCERA-1 down regulates pro-inflammatory cytokine (TNF, IL-12 and IL-23 p40) production and simultaneously up-regulates production of an anti-inflammatory cytokine (IL-10). In our continuous efforts [1-2] to understand the mechanism of action of PCERA-1, here we have developed an efficient synthesis that allows access to PCERA-1 photoaffinity probes from readily available starting materials (Fig 1). The probe contains a photoreactive group, a diazirine moiety, and a handle which will allow us to perform biorthogonal chemistry in order identify putative proteins that bind this highly active immunosuppressant.

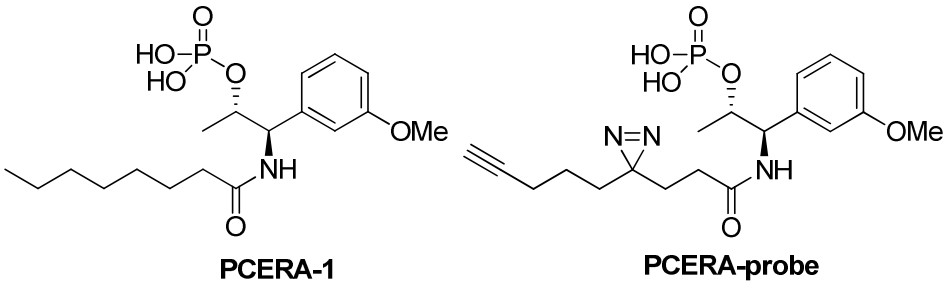


**Fig 1.** Structures of PCERA-1 and biomimetic tag-free photoactivatable probe.

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**O-33**

# Chemoenzymatic synthesis, nanotisation and anti-*Aspergillus* potential of novel fluconazole analogues

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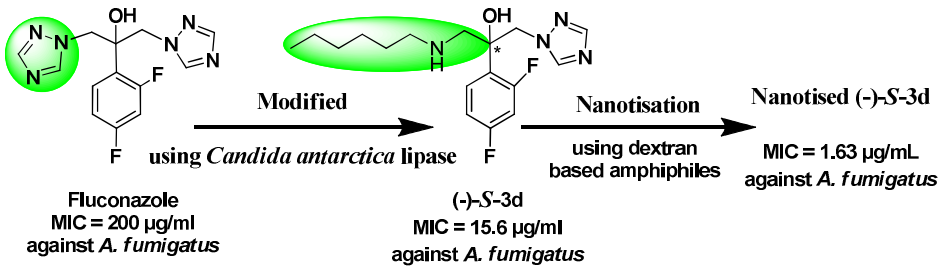
We report the first successful application of *Candida antarctica* lipase (CAL) for the preparation of optically enriched fluconazole analogs. Anti-*Aspergillus* activity was observed for the optically enriched derivative, *(-)-S*-2-(2',4'-difluorophenyl)-1-hexylamino-3-(1'",2'",4'") triazol-1'"-yl-propan-2-ol [*(-)-S*-**3d**], which exhibited an MIC value of 15.6 µg/mL and 7.8 µg/disc in microbroth dilution and disc diffusion assays, respectively. *(-)-S*-**3d**is well tolerated (up to 1000 µg/mL) by mammalian erythrocytes and cell lines (A549 and U87). When incorporated into dextran nanoparticles, the fluconazole analog *(-)-S*-**3d** exhibited improved antifungal activity (MIC = 1.63 µg/mL) against *Aspergillus fumigatus* and was better tolerated by human cells.




The results of these investigations shall be presented at the ISCB Conference.

**O-34**

# Green Approach for Synthesis of Bioactive Hantzsch 1,4-Dihydropyridine Derivatives Based on Thiophene Moiety via Multicomponent Reaction

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**Abstract:** A novel green and efficient one-pot multicomponent synthesis of dihydropyridine derivatives in good to excellent yield were reported. In presence of CAN catalyst, different 1,3-dione and same starting material as 5-bromothiophene-2-carboxaldehyde and ammonium acetate were used under solvent and heat free (at room temperature) condition for the Hantzsch pyridine synthesis within short period of time. All compounds were evaluated for their *in vitro* antibacterial and antifungal activity and interestigly we found that **5b** to **5f** shows excellent activity than Ampicilin, whereas only **5e** compound shows excellent antifungal activity against *C.albicans* compared to graseofulvin. The cyto-toxicity of all compounds has been assessed against Brest tumor cell lines (BT-549) but no activity was found. The X- ray structure of one such compound **5a** viewing colourless block crystal was corresponded accurately to a primitive monoclinic cell.

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**O-35**

## Micellar catalysis a greener approach in pharmaceutical industry

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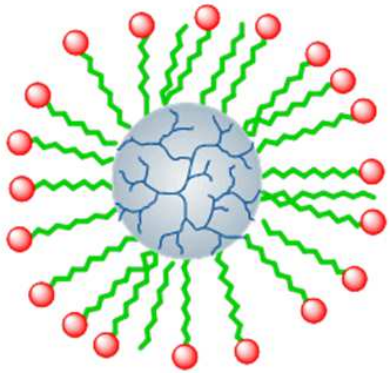
Green chemistry, is also called sustainable chemistry, it is a philosophy of chemical research and engineering that encourages the design of products and processes that minimize the use and generation of hazardous compounds. The most simple and direct way to apply green chemistry in pharmaceuticals is to utilize ecofriendly, nonhazardous chemical and also minimize or replace the use of toxic solvents from pharmaceutical processes.Now a days industries are constantly challenged to think about more environmentally benign, scalable and cost effective process in various industriesespecially in pharmaceutical industries. As a result, green chemistry has attained the status of major scientific discipline, leading to the development of cleaner and green process. The use of surfactant in pharmaceutical development is the emerging area. Surfactants in water play a dual role both as catalyst to activate the substrate molecule and as surfactant to increase the localized concentration of organic reactants to form micelles in water which enable the various organic transformations at normal temperature.



**Nano micelles**

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O-36

# PHARMACOKINETIC STUDY OF AMINO ACID PRODRUG OF GLICLAZIDE BY LC-MS/MS METHOD IN RABBIT PLASMA

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**Abstract:** Amino acid prodrug of gliclazide is a water soluble and biologically inactive derivative of gliclazide, a sulphonyl urea analogue used to treat type II diabetes mellitus. A rapid liquid chromatography tandem mass spectrometry LCMS-MS method has been optimized for analysis of amino acid prodrug of gliclazide in rabbit plasma using clopidogrel as internal standard. Following turboionspray ionization, the analytes were quantified on a triple–quadrupole mass spectrometer in multiple-reaction-monitoring (MRM) positive ion mode. Sample preparation involved a simple one-step protein precipitation with methanol, followed by centrifugation and evaporation of the organic solvent. The residue was redissolved in mobile phase and analyzed by LC–MS/MS. A Symmetry C18, 50x4.6, 5µ, a mobile phase composed of Acetonitrile: 25mM Potassium dihydrogen orthophosphate (pH-6.5) (50:50 v/v), and a flow rate of 0.6 mL/min were employed, and the total run time was 3.0 min. The method was validated for accuracy, precision, linearity, selectivity, lower limit of quantification (LLOQ), recovery and matrix effect. The method was found to be linear in the range of 150 to 6000ng/mL. LLOD and LLOQ was found to be 8ng/mL and 25ng/mL respectively. All validation parameters met the acceptance criteria according to regulatory guidelines.This methodwas successfully applied to pharmacokinetic study of the prodrug in rabbit through oral administration.

**Keywords:** Amino acid prodrug, gliclazide, LCMSMS method,validation, pharmacokinetic study

**O-37**

# Synthesis of 3-Aroylimidazo[1,2-*a*]pyridine, and Functionalization of Imidazo[1,2-*a*]pyridines using Vanadium Catalyst

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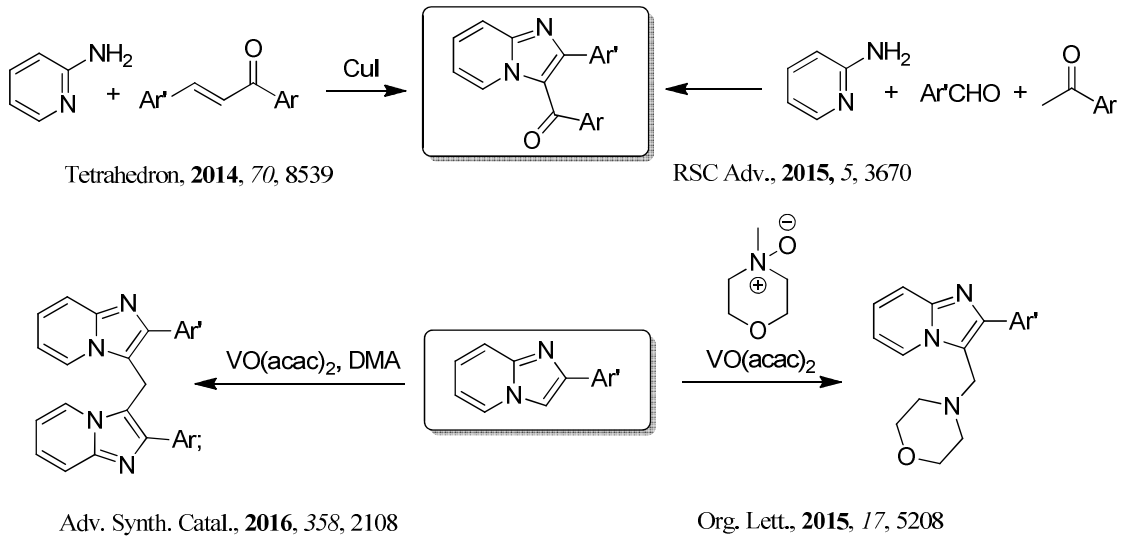
Imidazo[1,2-*a*]pyridine, a bicyclic *N*-fused imidazole, is an important molecule present in several pharmacologically relevant structures, and have shown many biological activities such as anti-bacterial, anti-ulcer, anti-viral and anti-inflammatory.[1] Zolpidem, alpidemzolimidine and saripidem are some important drug molecules which contain imidazo[1,2-*a*]pyridine skeleton.Recently, 3-aroylimidazo[1,2-*a*]pyridines has been proved as anticancer and antitumor agent.[2]We have been involved in the development of simple and mild methods for the synthesis and functionalizationof this biological important motif*via* C−H bond activation using different transition metal catalysts.[3] A brief overview of the work towardssynthesis of 3-aroylimidazo[1,2-*a*]pyridines, and functionalization of imidazo[1,2-*a*]pyridinesusing vanadium catalyst will be presented (Scheme 1).

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**Scheme 1**

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**O-38**

# Advanced Approaches of Green Principles to Achieve Sustainability of Modern Domestic life

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Green Chemistry is a modern science of chemistry. It is a Knowledge and analysis of the think of products or substance which are not involve materials adverse to the environment and also it extent with the utilization of ecofriendly chemical compounds in different region of our life such as industrial, agriculture uses and many others. Green chemistry was developed by the need of to skip out organic and inorganic chemical which are hazardous to living organisms. It plays important role in deciding the nature of best modern life. Most of the pharmaceutical, chemical industry and other related industries produce us with extremely mixed bag of crucial products of plastics to pharmaceuticals these are responsible for serious damage of environment. To protect the environment from hazardous chemical compounds two scientists proposed Anastas and Warners 12 principle for green chemistry. Those principles explain cleanup the waste after it has been created, maximize the product in synthesis, in synthetic process using chemicals will produce less toxic effects, newly designing compounds must be minimize the toxic effect, And use safer solvents, renewable feed stock, design easily degradable material in synthesis. Along this principles some of developed techniques will be protect the environment from various factors. The Present work explains application of green chemistry principles in everyday life especially reuse of domestic materials effectively to attain sustainability.

**Key words:** Benign chemistry, Environmental sustainability.

**O-39**

## Design, Synthesis in silico high throughput screened and discovery of novel human p-glycoprotein inhibitors as MDR cancer

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P-glycoprotein or permeability glycoprotein (Pgp) is an ATP dependent efflux pump protein belonging to a family of ATP binding cassette (ABC) transporters involved in unidirectional pumping of Xenobiotic out of the cell. P-gp expression causes drastic reduction in intracellular drug concentrations which results in decreased cytotoxicity of a wide range of anticancer drugs. Therefore, multidrug resistance in cancers can be overcome by P-gp inhibition. Numerous P-gp inhibitors have been isolated or chemically synthesized for modulating activity MDR in cancers but these efforts have been limited by unwanted immunosuppressive and cardiovascular toxicity. The current study reports 22 novel hybrid molecules containing the 1, 2, 3 triazole and dihydropyrimidine core, synthesized based on the P-gp binding site. The synthesized compounds were further screened against the computational model of human P-glycoprotein, predicted using the multiple template based comparative modeling approach and subjected to 50ns MD simulation, energy minimization and structure optimization to identify the most stable conformation. Based on the QM/MM docking study, the amongst all 22 compound 6ad found to have better binding affinity towards P-gp than the known inhibitor Verapamil. This was further validated by free energy landscape binding study. Furthermore, P-gp inhibition assay and MTT assay for growth inhibition unveil that 6ad showed three-fold higher activity than the first line and second line inhibitor of P-gp. Additionally, ADME/Tox prediction and DFT study for HUMO-LUMO calculation results also showed that 6ad displayed stronger drug like profile better reactivity than verapamil and also less Insilco toxicity profile. However, this would require further in-vitro validation study to decipher the exact mechanism of action and the pathway targeted by 6ad. These results indicate that 6ad is a novel lead for the development of next generation Human P-glycoprotein inhibitor

**O-40**

# First Total Synthesis and Biological Potential of a Heptacyclopeptide of Plant Origin

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**ABSRACT:** Medicinal plants have been used to treat health disorders and to prevent diseases since time immemorial. [1] Recently, the World Health Organization has estimated that 80% of people worldwide rely on herbal medicines for some part of their primary health care. Natural products from medicinal plants provide unlimited opportunities for new drug leads because of the unmatched availability of chemical diversity. [2] Plant-derived cyclopeptides have complex structures with modified and/or unusual amino acid moieties and are concerned with a number of bioactivities including antifungal activity, insecticidal activity, tyrosinase inhibitory activity, anthelmintic activity, anti-inflammatory activity, vasorelaxant activity, estrogen-like activity, antimalarial activity, anticancer activity. A natural cyclic heptapeptide - mahafacyclin A with $\beta$-bulge characteristics, has been isolated from *Jatropha mahafalensis* latex and its structure was elucidated by a combination of chemical degradation, LSIMS data and 2D NMR experiments. Minute quantities of this bioactive cyclopeptide obtained from natural resources (328 mg from 250 g of dry latex of *J. mahafalensis*) restricted scientists to investigate its biological profile in detail. Synthesis of a natural glycine-rich heptacyclopeptide - mahafacyclin A was accomplished by solution-phase technique of peptide synthesis *via* coupling of tetrapeptide unit Boc-*L*-Thr-*L*-Ile-*L*-Leu-Gly-OH with tripeptide unit *L*-Val-*L*-Phe-Gly-OMe followed by cyclization of linear heptapeptide fragment. Structure of newly synthesized cyclopolypeptide was confirmed by means of chemical, spectroscopic analyses and subjected to antibacterial, antifungal and anthelmintic activity studies. Bioactivity results showed potent antifungal and anthelmintic activities of synthesized peptide against dermatophytes *T. mentagrophytes*, *M. audouinii* and earthworm species *M. konkanensis*, *P. corethruses* and *E. eugeniea*.

**Keywords:** *Jatropha mahafalensis*, peptide synthesis, cyclopolypeptide, natural product, pharmacological activity

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**O-41**

# Triflic anhydride mediated room temperature Synthesis of 3-substituted Benzofurans

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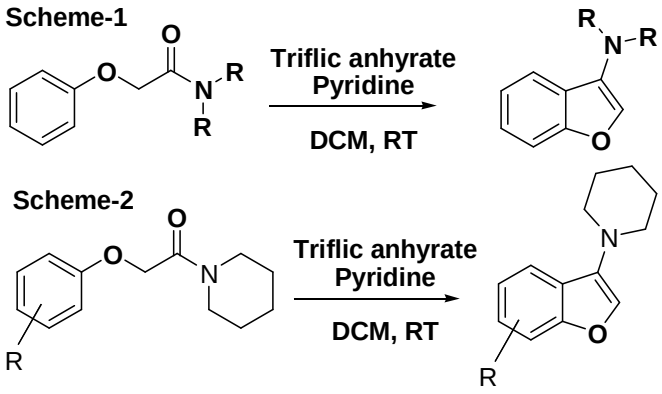
Benzofuran ring is a common structural element that appears in a large number of medicinally important compounds [Yoo et al]. The benzofuran nucleus is widely distributed in natural products particularly among plants. In the chemistry of benzofurans in a large number of natural products has attracted due to their biological activities and their potential application as pharmacological agents [Bakr et al]. In continuation of our studies on synthesis of biologically significant Benzofuran derivatives. We present here a room temperature Triflic anhydride and Pyridine mediated cyclization of N,N-dialkyl-2-phenoxyacetamides into *N,N*-dialkylbenzofuran-3-amine derivatives and substituted 2-phenoxy-1-(piperidin-1-yl)ethanone into 1-(benzofuran-3-yl)piperidine benzofurans derivatives is disclosed. This efficient method leads to the formation of biologically essential 3-Substituted benzofurans in good to excellent yields. The remarkable advantages of this method over conventional heating are decreasing reaction times and increasing yields, formation of products in analytically pure form, operational simplicity less energy consumption make this protocol cost-effective and environmentally more benign. We believe that this approach is quite useful to synthesize 3 substituted benzofurans.

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**O-42**

# Synthesis and Characterizationof Sodium Salt of Carboxymethylated Sodium Alginate graftedPoly (methyl acrylate)

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**ABSTRACT:** Potassium Persulfate mediated grafting of poly(methyl acrylate) (PMA) onto Sodium Salt of Partially Carboxymethylated Sodium Alginate (Na-PCMSA) in an aqueous medium under nitrogen atmosphere was studied and the optimum reaction conditions with respected to the concentrations of initiator (CAN),nitric acid monomer & amount of substrate as well as reaction time & temperature were evaluated in terms of percentage of grafting(%G) and percentage of grafting efficiency(%GE). All the products were characterized by spectroscopic (IR) and scanning electron microscopic (SEM) techniques.

# POSTERS

P-1

# SELENIUM DIOXIDE ASSISTED α, α- DIARYLATION OF BRANCHED ALIPHATIC KETONES IN PRESENCE OF PARATOLUENE SULFONIC ACID: A NOVEL METHOD FOR THE SYNTHESIS OF 1, 1-DIARYL ALKYL-2-ONE

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The addition of an aryl group to the α-carbon of a carbonyl compound is one of the important reactions in organic synthesis as this reaction can effectively form C-C bonds to provide valuable molecules that are the core structures of natural products or pharmaceutical. Many methods have been developed for the synthesis of arylated compound involving the use of palladium-based catalysts. Arylation of activated methylene compounds mediated by copper salts and proline has also been achieved in presence of CuI. We report here a simple and an efficient method for the synthesis of 1, 1-diaryl alkyl-2-ones via the α,α-diarylation of branched aliphatic ketones using selenium dioxide in the presence of para-toluene sulfonic acid.

**P-2**

# Design, Multicomponent Synthesis and Characterization of Diversely Substituted Pyrazolo[1,5-a] Pyrimidine Derivatives

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The synthesis of various heterocyclic compounds using acetoacetanilide[AAA], we have demonstrated that acetoactanilide are versatile intermediate for the synthesis of pyrazolopyrimidine derivatives. Thus, to explore further, we sought that the reaction of various acetoactanilide, an appropriate aldehyde and 5-amino-*N*-cyclohexyl-3-(methylthio)-1*H*-pyrazole-4-carboxamide in the presence of base in isopropyl alcohol could be an effective strategy to furnish the novel pyrazolopyrimidine derivatives. Here we describe the novel synthetic methodology for the fused pyrazolopyrimidines.

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**P-3**

# One-Pot Sequential Approach for the Construction of Highly Functionalized Triazolo[4,3-c]pyrimidine Library

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Novel [1,2,4]triazolo[4,3-c]pyrimidine-8-carboxamides were synthesized via oxidative cyclization of hydrazono-1,6-dihydropyrimidine-5-carboxamide intermediates by the application of iodobenzenediacetate as a sole cyclizing agent. Here, we report a one-pot sequential strategy to generate the corresponding triazolopyrimidines by condensation of preprepared a-acylketenedithioacetals and arylamidines. Moreover, this process describes the application of presynthesizedarylamidines, which omits the Suzuki–Miyaura cross-coupling reaction and hence provides metal-free organic synthesis in an atom- and step-economical fashion

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**P-4**

# Tetrahydrobenzo thiazole and triazole hybrid heterocyclic compounds:Design, Synthesis and characterization study

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**Abstract:** A series of new 4,5,6,7-tetrahydro-1,3-benzothiazolesbearingtriazole ring were synthesized. We have designed the synthesis route in five steps starting with bromination of cyclohexanone using NBS (N-bromosuccinamide). Followed by there are common different reaction phenomenonused in the reaction scheme. In the last step DCC (N,N'-Dicyclohexylcarbodiimide) was used for the purpose of an amide coupling. The use of DCC is shortening the reaction time as well as easy to workup of the reaction and giving good yield in the range of 50-65%.

**Key words:** cyclohexanone, NBS, 4,5,6,7-tetrahydro-1,3-benzothiazole, triazole, DCC, amide coupling.

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P-5

# Computational design of repeat units for potential information-bearing macromolecular H-bonded duplexes, Part I. Polyamide backbone

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**Abstract:** Repeat units for DNA-like potential information-bearing polymeric H-bonded duplexes are designed here by assigning a suitable backbone structure to a set of 4 pyrimidine bases which can form 2 H-bonded base pairs. Each strand of the proposed duplex has the structure (-NH -$CH_2$-CH**B**-CO-)$_n$ or (-CO-CH**B**- $CH_2$NH-)$_n$, where **B** is a pyrimidine base, so that the backbone may be described as having a polyamide structure. The monomeric repeat units may be described as $NH_2$- $CH_2$- CH**B**-COOH which may combine successively by N-C peptide bond formation through loss of $H_2O$ to give the polymeric single strand. Two complementary monomeric repeat units can pair through H-bonding to yield a backboned pair. Density functional theory at the wB97XD/6-311++G(d,p) yields optimized structures for the 4 monomeric repeat units. *Antiparallel* and *parallel* type of backbone orientations are considered which yields four stable backboned pairs. The calculated pairing energies predict sufficient stability of the H-bonded pairs. The four H-bonded pairs are predicted to be isomorphic, suggesting a periodic structure for the putative H-bonded macromolecular duplex.

**Keywords:** H-bonded nitrogenous base pairs · information-bearing · macromolecular duplex ·isomorphic base pairs · density functional theory.

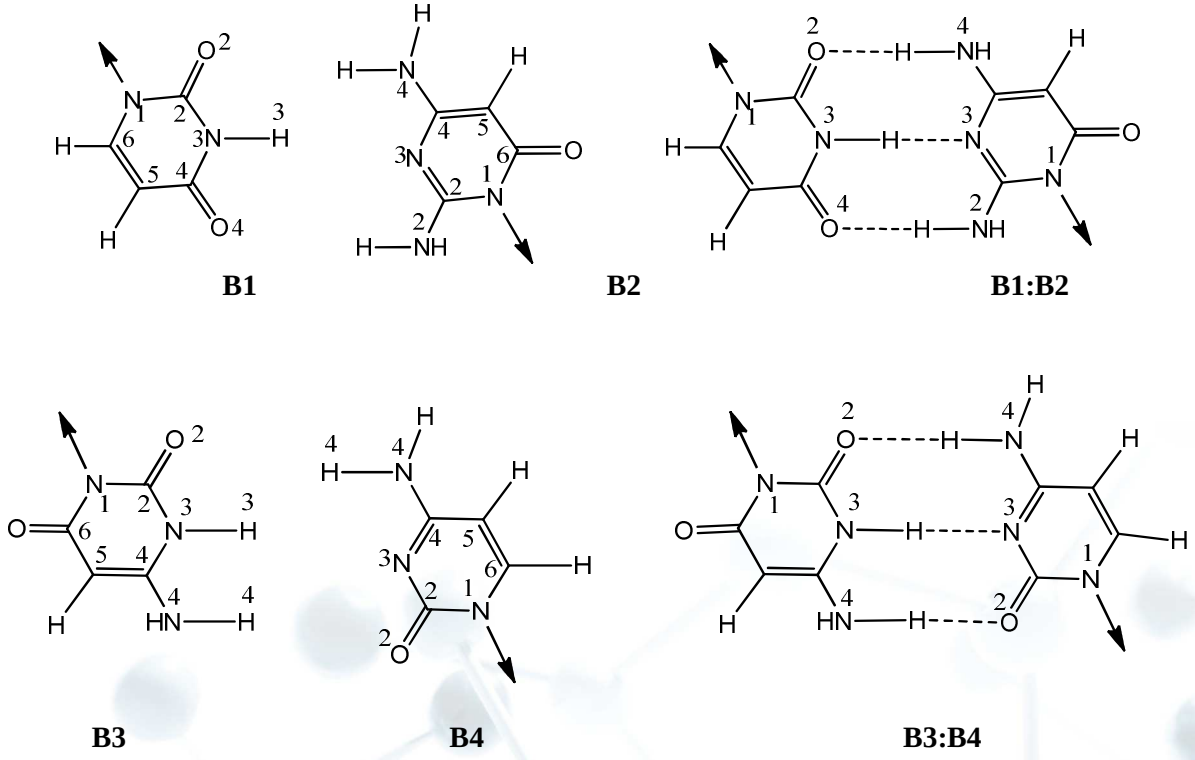


**Fig 1.** Component bases **B1**, **B2**, **B3** and **B4** and the base pairs **B1:B2** and **B3:B4**

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**P-6**

# Design, Synthesis and Characterization study of New Tetrahydrobenzo Thiazole Containing Pyrimidine Via Biginelli Approach

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**Abstract:** Thiazole moiety is a core constituent of many pharmacologically important synthetic and naturally occurring drugs. In addition, thiazoles are an interesting class of heterocyclic compounds that possess potentactivities such as antimicrobial, antitubercular, anti *HIV*etc. In view of the previously mentioned findings and in continuation of our work aimed at the synthesis of a variety of heterocyclic ring systems for biological and pharmacological evaluation, we report here in an efficient method for synthesis of some new 4,5,6,7-tetrahydro-1,3-benzothiazoles bearing pyrimidine ring. Thiazole is versatile building blockfor the synthesis of awide variety of severalthiazole-based heterocyclic derivatives. We have designed the synthesis route in five steps, starting with bromination of cyclohexanone using NBS (N-bromosuccinamide), followed by reaction of 4,5,6,7-tetrahydro-1,3-benzothiazoles amide with active methylene compound, gave acetoacetanilide of this amine which onfurther reaction with aryl aldehyde and thiourea to gave4,5,6,7-tetrahydro-1,3-benzothiazoles-2-thioxo-4-aryl-1,2,3,4-tetrahydro pyrimidine-5- carboxamide. This synthetic approach has various prominent features such as good yield in the range of 85-90% and simple reaction condition and easy purification process.

**Key words**: cyclohexanone, NBS, acetoacetanilideand aryl aldehyde.

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**P-7**

## Synthesis and Characterization Fluorinated carboxamides derivatives as anticancer agents

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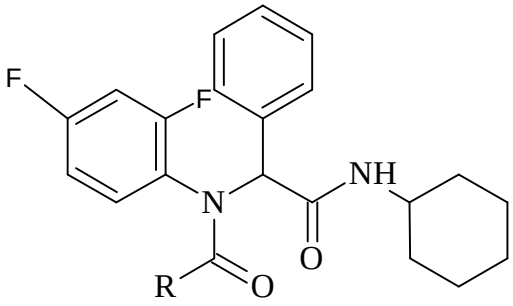
As per current scenario, Ugi reaction is an established route for atom economy to synthesis pharmaceutically active component.Flouro substituted carboxamides motif itself possesses a variety of biological function.On other side in the field of medicinal chemistry many other heterocycles containing fluoro substituted motif were also known for their prominent impending against different cancer cell line.In particular, anticancer research has been capitalizing on the intrinsic versatility and dynamic core scaffold of these compounds. From the above cited literature review, we have synthesized carboxamides derivatives bearing flouro substituted amine and evaluated for their anti-cancer activity.




The Characterization of all the synthesized compounds done by NMR and IR spectroscopic methods. Further supported by Mass spectrometry.

**P-8**

# Efficient synthesis of substituted benzofuran derivatives via friedel craft reaction

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**Abstract:** In recent years much interest has been focused on the chemistry of Benzofuran and their derivatives, which are presented as valuable substituents for substituted benzofuran drugs, clinically used in the treatment of various diseases.

The purpose of the present work is to explore the synthetic potential of these compounds in order to construct new substituted benzofuran derivative as a potential anti arrhythmic, anti cancer, and anti tubercular agent. The chemistry of oxygen hetero atom containing aromatic compounds is becoming more popular as an area of research among the present day chemists. Hence the increasing trends in the study of such compounds and its versatile activity like anti arrhythmic, anti cancer, anti hypertensive and anti tubercular etc, the present work of synthesis of substituted benzofuran derivatives as undertaken.

The desired compounds were prepared using simple starting materials like 2-(bromomethyl)-4-nitrophenol and pentanoyl chloride. Followed by friedel craft reaction of this benzofuran compound with 4-methoxy benzoyl chloride to get substituted benzofuran which on demethylation followed by reaction with triflic anhydride to get triflate of respected compound which on sonogashira reaction with trimethyl silyl to get our scaffold which on copled with different aryl iodide to get our final product.

**Key Words:** Benzofuran, Pentanoyl chloride, Friedle craft Reaction, Triflic Anhyride, Sonogashira Reaction.

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**P-9**

# Synthesis and characterization of some new N-substituted spiroindole derivatives

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**Abstract:** Hetrocyclic carbonyl compounds are of great interest since they exhibit numerous biological activities such as antitumor, antimicrobial, antibacterial activity etc. Spiroindole are one of the most biologically important molecules. In present work we have reportedspiro (indoline-3,3'-pyrrolidin)-2-one which is synthesized by 2-(1*H*-indole-3-yl) ethane-1-amine and glyoxalic acid. During synthesis we have used Cbz as a protecting group to avoidunwanted product formation. In the scaffold there aretwonitrogen,so we have synthesized two different N-substituted compound series using different aryl benzoyl chloride.

**Keyword**: indole derivatives,glyoxalinc acid, Cbz, 2-(1*H*-indole-3-yl)ethane-1-amine.

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**P-10**

# Molecular Docking And ADMET Studies Of Some Novel 1,2,4- triazoles As Lanosterol 14-alpha-demethylase Inhibitors

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**Abstract:** Today there is a considerable increment in the application of *in-silico* molecular modelling and docking studies to predict potential inhibitors (drugs) for the treatment of several diseases. Further ADMET prediction has become increasingly important in drug design and development. Lanosterol 14 alpha demethylase, a microsomal cytochrome P-450-dependent enzyme impair the biosynthesis of ergosterol which is an important target for novel antifungal drugs. Owing to the biological importance lanosterol 14-alpha demethylase inhibitors, thirty five compounds having 1,2,4, triazole have been collected from the literatures and their binding affinities towards lanosterol 14-alpha demethylase enzymes were checked through molecular docking studies. GLIDE Integrated Maestro 9.3 version was used. All the compound showed more affinity towards the enzyme Lanosterol 14 alpha demethylase, particularly three compounds namely ***9-(3"-methyl)-3-(4'-nitrophenyl)-5H,13aH-quinolino[3,2-f][1,2,4]triazole-[4,3-b][1,2,4]triazepine,3,6-diamino-[1,2,4]triazolo[4,3-f][1,2,4]triazin-8(7H)-one, 3-(N-4'-chlorophenylcarboxamidoethylthio)-4H-1,2,4-triazole*** showed better results than the standard ketoconazole. However these compounds may be further investigated for their lanosterol 14-alpha demethylase inhibitory activities through suitable *in-vitro* models. ADMET studies were performed by using Qik prop version of Schrodinger 2011. They showed satisfactory results.

**Keywords:** Lanosterol 14-alpha-demethylase, Triazoles, ergosterol biosynthesis.

**P-11**

# EVALUATION OF ANTIOXIDANT, ANTIMICROBIAL AND CYTOTOXICITY STUDIES OF SIDA CORDIFOLIA LINN

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**Abstract:** The Indian system of medicine, Ayurveda, medicinal science practiced for a long time for disease free life. It relies mainly on the medicinal plants (herbs) for the management of various diseases /ailments. Few plants are still used as the richest source of medicine since the age. Sida cordifolia linn is one of such plants, which is being used in the medicine of Ayurveda. The goal of this work was to screen traditionally used sida cordifolia for anti-oxidant, antimicrobial, cytotoxicity studies. The expectation that some naturally occurring plants compound can kill antibiotic-resistant strains of bacteria such as Bacillus cereus, Escherichia coli, Micrococcus luteus and S. Aureus were been confirmed. The anti-microbial activity of the crude extracts were checked against various gram positive and gram negative microorganism and also some of the fungal stain were determined by cup plate method and minimum inhibitory concentration methods. In antioxidant studies, among the extracts methanolic extract showed the maximum activities for DPPH and Nitric oxide method. The cytotoxicity data showed that the methanol extract of Sida cordifolia possessed highest toxicity at a concentration of 30.69µg/ml against breast cancer cell line.

**Key words:** Sida cordifolia, Escherichia coli, antioxidant, antimicrobial, nitric oxide, DPPH, methanol extract.

**P-12**

# Synthesis, characterization, and Antimicrobial Activity of Some new N-acetyl Pyrazoline derivatives from Chalcones

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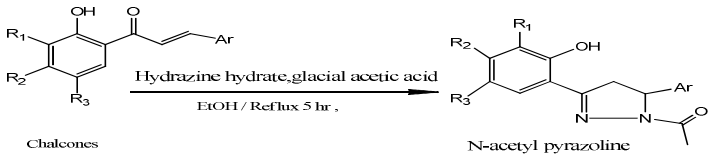
**ABSTRACT:** Pyrazolines are novel class of 5-membered heterocyclic compounds possessing wide variety of biological and physiological activities .These activity due to present of a nitrogen atom. Which is stimulating the research activity in this field.Amongst these, N-acetyl Pyrazolines are well known and important nitrogen conaining five membered heterocyclic compounds. Several N-acetyl pyrazoline derivatives have been found to possess considerable biological activities such as anticancer,[1-2] anti-inflammatory,[3-5] analgesic and antipyretic,[6] antimicrobial,[7-8] and anti-tubercular agents.[9]1,3-diaryl prop-2-en-1-one very well known as Chalcone, is the molecule which was known from many decades due to its wide range of biological activities such as antimicrobial, anti-inflammatory, analgesic, antiplatelet, antiulcerative, antimalaria, anticancer, antiviral, antileishmanial, antioxidant, antitubercular, antihyperglycemic, immunomodulatory, chemical mediators release inhibitors , leukotriene B4 inhibitors , tyrosinase inhibitors and aldose reductase inhibitors activities. Chalcones belongs to falvanoid family and present in various plant species such as fruits, vegetables, spices, tea etc. Chalcones are intermediate for the synthesis of number of heterocycles for eg. Pyridine, pyrimidine, pyrazoline, isooxazoline, flavanoid, benzodiazepine, indazole, azetidinone which also shown various pharmacological activities.

**KEYWORDS:** N-acetyl Pyrazoline, Synthesis, Antibacterial activity, Antifungal activity.

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# Central Composite Design Approach for Robustness Testing Of HPTLC Method for Simultaneous Determination of Stavudine and Lamivudine in Pharmaceutical Formulation

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**Abstract: Oblective:** A High Performance Thin Layer Chromatographic method (HPTLC) for the simultaneous estimation of Stavudine (STD) and Lamivudine (LAD) was optimized and validated as per ICH guidelines. Robustness testing performed by using Central Composite Design (CCD). **Material and Methods:** Namita Kapoor et al. [1], Jayakar B et al. [2], Gholamreza B et al. [3], SrivaniMallepelli ei al. [4] HPTLC separation carried out by using plates pre-coated with silica gel $60F_{254}$ and Acetonitrile: Ethylacetate: Water (6:3:1v/v/v) as a mobile phase. The detection wavelength for simultaneous estimation of both the drugs was 254nm (isosbestic point). **Result:** The $R_f$ values for STD and LAD were 0.20 and 0.60 respectively. Percent recoveries of the marketed formulation were found to be 98.17-100.2, 99.21-102.9 for STD and LAD, respectively. The obtained value for repeatability studies and intermediate precision was found to be less than 2% of percentage relative standard deviation for STD and LAD, respectively. All the three factors evaluated in the robustness testing by CCD Umesh M Patel [5], were found to have an insignificant effect on the retention factor. The content of acetonitrile in total mobile phase as a factor involved having a significant effect on robustness when compared to band size and developing distance and it is necessary to be carefully controlled. Srinubabu G et al [6], Srinu babu G et al [7] **Summary**: simple, accurate and reproducible HPTLC method was developed, which would be of use in routine quality control for the marked formulation. Harang V ei al [8].

**Keywords:** Central Composite Design, High Performance Thin Layer Chromatography, Lamivudine, Stavudine, Validation.

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**P-14**

# Preparation and Characterization of Tangeritin as Solid-Lipid Nanoparticles (SLNs)

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**Abstract: Introduction:** Tangeritine is a O-Methylated Isoflavone which possess many pharmacological effect but due its poor oral bioavailability (3%) and extensive first pass metabolism along with biliary elimination, the action of Tangeritine is drastically reduced (Wahajuddin *et al*., 2011) **Aim:**Solid-Lipid nanoparticles are well tolerated lipid carrier system due to the employment of biodegradable lipid matrix (Shahul *et al*., 2014) The present research work is carried out to preparation and evaluate the Tangeritine solid-lipid nanoparticles (SLN) which enhances the solubility, improved bioavailability. **Method:** Tangeritine-SLN were prepared with stearic acid (lipid) tween 80, span 20 by solvent injection method (Kaushik *et al*., 2012) Tangeritine-SLN were characterized by Fourier Transform Infrared Spectroscopy (FTIR), Mean Particle Size, Scanning Electron Microscopy (SEM), Zeta Potential, Entrapment Efficacy and invitro drug release (Silpa *et al*., 2012) **Results:** From the results, Tangeritine has been successfully prepared as Solid-Lipid Nanoparticles which helps in overcoming its drawbacks.

**Keywords:** Tangeritine, Solid-Lipid Nanoparticles, Solvent Injection Method

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**P-15**

# Silica Nanosphere-Graphene Oxide ($SiO_2$ -GO) Hybrid Catalyzed Facile Synthesis of Functionalized Quinoxaline Derivatives

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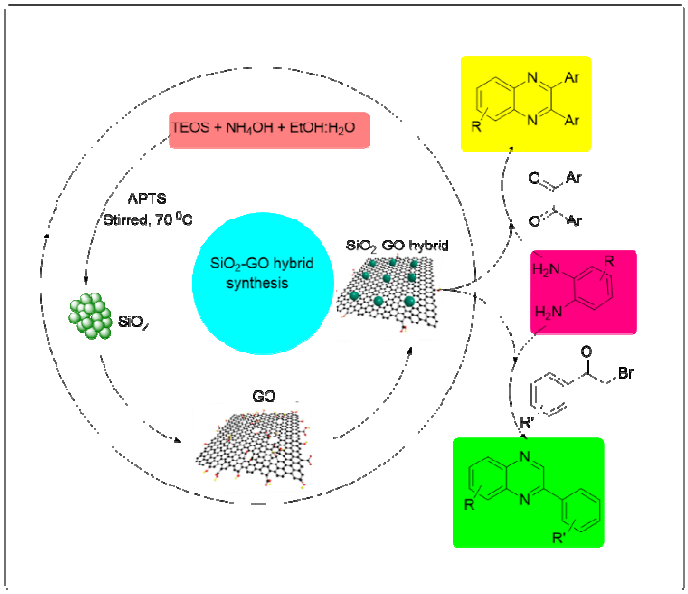
Spherical $SiO_2$ nanoparticles (5±0.2 nm) excellent with unifirm size and even distrubation were prepared on graphene oxide ($SiO_2$-GO) by using simple *in situ* one step method. Transmission electron microscopy (TEM) and other spectroscopic characterization demonstrated that GO acted as a good supportive substrate for controlling the size and activity of $SiO_2$ nanospheres from their cooperation towards catalytic reactions. The optimized hybrid exhibited high catalytic activity for the synthesis of functionalized quinoxalines. Significantly, as-synthesised $SiO_2$-GO nanohybrid catalysed reaction was shown to be highly efficient in mild condition (i.e. room temperature, air), with excellent product yield (92%) and good recyclability (upto 4 cycles) at room temperature for the first time.

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P-16

# Experimental design to develop a robust UPLC method forQuantification of p-phenylenediamine in Cosmetic Preparations

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**Abstract:** A simple and reproducible UPLC method was developed and validated for the quantitative analysis of p-phenylenediamine (PPD) in cosmetic preparations. Method validation demonstrated the reliability and consistency of analytical results. Central Composite design (CCD) withthree factors and one response was employed to study the robustness of the developed method.The developed method was examined forvalidation parameters like linearity, specificity, precision, accuracy and robustness. The method was found linear over a wide range of 5.0 – 400 µg/ml with a regression coefficient of 0.999. The %RSD for Precision studies (Inter and Intraday) was found NMT 2 %. Extraction efficiency of 98% was obtained. Accuracy, ascertained by employing % Recoverywas calculatedand found between 98-103 % w/w. CCD generated and carried out proves the method developed wasrobust.All the validation parameters were reported to be within the acceptance limit. The content of PPD in 20 different cosmetic preparations available in local markets in and around Chennai was ascertained. Theproposed and developed UPLC method was applied for routine analysis of PPDin cosmetic preparations and can also be extended to theanalysis in pharmaceuticals and food products.

**Keywords:** p-phenylenediamine (PPD), Central Composite design, UPLC, Cosmetics preparations.

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**P-17**

## Qualification and Quantification of impurities from biologically active drugs

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Presence of unwanted chemicals, even in small amounts, may influence the efficacy and safety of the pharmaceutical products. Therefore impurity profiling (i.e.,the identity as well as the quantity of impurity in the pharmaceuticals), is receiving critical attention from regulatory authorities.Various regulatory authorities such as the International Conference on Harmonization (ICH), the United States Food and Drug administration (FDA), and the Canadian Drug and Health Agency (CDHA) have been legally emphasized on the purity and the identification of impurities in Active Pharmaceutical Ingredients (APIs)[1]. However, it is noted that large number of compounds under investigation in drug discovery presents a significant analytical challenge for the detection, quantitation, and characterization of the compounds alone Pilaniya *et al.* [2].

Chromatography is one of the quickest and easiest ways to separate complex mixture of compounds. The present work defines the application of flash / preparative chromatography instrument with auto fraction collector for separation of impurities present in active drug molecules and various isomeric agrochemicals. The isolated impurities were further quantified and qualified by sophisticated analytical instrumental techniques such as Infra-Red (IR),Nuclear magnetic resonance ($^1$H-NMR), High performance liquid chromatography (HPLC) and Mass spectroscopy (MS).The efficiency of purification was confirmed by achieving 97-99% purity of the active molecules.This reproducible analytical technology has been consistently represented the accurate, high throughput, robustresults in impurity identification,detection,and quantification for variety of drug molecules. We envision that this impurity profiling information on biologically active molecules would help thepharma industries to speed up the developmental stage of drug candidatesfrom IND to NDA.

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**P-18**

# EVALUATION OF ANTI PARKINSON'S ACTIVITY OF HYDROALCOHOLIC EXTRACT OF *Acoruscalamus*

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**ABSTRACT:** Parkinson's disease (PD also known as idiopathic or primary Parkinsonism, hypokinetic rigid syndrome/HRS) is a degenerative disorder of the central nervous system. Modern treatments are effective at managing the early motor symptoms of the disease, mainly through the use of levodopa and dopamine agonists. As the disease progresses and dopaminergic neurons continue to be lost, these drugs eventually become ineffective at treating the symptoms and at the same time produce a complication called dyskinesia, marked by involuntary writhing movements. *Acoruscalamus*, a traditional herbal plant shows anti-cholinergic effects which can be used as a pathway for treating Parkinson's disease.[1] The aim and objective of this study is to investigate the anti-parkinsonian effect of*Acoruscalamus*. Oxotremorine antagonism is brought about by the injection of Oxotremorine and the effect of *Acoruscalamus* is studied by evaluating the locomotor activity [2], tremor, hyperkinesia and rigidity of the mice [3-4] and the biochemical parameters.

**KEY WORDS:** Parkinson's disease, Oxotremorine, Hyperkinesia, Tremor, Biochemical parameters

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**P-19**

# Studies in synthesis and evaluation of hydrophilic and hydrophobic nanosized chitosan derivatives as potential sequestering agents for waste water management

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Water is an essential pharmaceutical aid; good quality of water is an important requirement for maintaining the healthcare of society. It is the most widely used substance, raw material or starting material in the production, processing and formulation of pharmaceutical products. Important challenges in the global water situation, mainly resulting from worldwide population growth and climate change, require novel innovative water technologies in order to ensure supply of drinking water and reduce global water pollution. Chitosan has gained inclusive attention as effective biosorbents due to low cost and high contents of amino and hydroxyl functional groups which show significant adsorption potential for removal of numerous aquatic pollutants Wang *et al.* [1].

The objective of this study is to evaluate hydrophobic and hydrophilic derivatives of chitosan for sequestration properties to remove broad range of inorganic (As, Cd, Cr, Co, Cu, Pb, Ni, and Zn) and organic (polycyclic aromatic hydrocarbons or textile dyes) from the polluted waste water. The present work deals with chemical modification of chitosan through alteration in the amino or hydroxyl functional groups with two main aims: (a) To improve metal sorption properties and (b) To alter the solubility of chitosan in water at different environmental pH conditions. The synthesized derivatives were characterised by FTIR, $^{1}$H-NMR, TGA and DSC. Since the sequestration of metal ions is dependent on the surface area, reduction in size or nanoscaling will increase the efficiency of adsorption Gehrke *et al.* [2]. This allows the development of novel high-tech materials for more efficient wastewater treatment.

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P-20

# EVALUATION OF IN-VITRO ANTIOXIDANT ACTIVITY OF ETHANOLIC EXTRACT OF UGLI FRUIT

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**ABSTRACT:** Medicinal plants are rich sources of natural antioxidants which are used in the prevention and treatment of diseases like artherosclerosis, heart stroke, diabetes, cancer and to delay the process of aging. Antioxidants are the chemicals which scavenge the free radicals and help in preventing and treatment of several diseases. Human body produces oxygen free radicals and other reactive oxygen species (ROS) as by products through numerous physiological and biochemical processes. *Citrus reticulate x Citrus paradise* ( Family: Rurtaceae) commonly known as Mandarin Orange or Loose- Skinned Orange is an edible fruit which is created by hybridizing a grapefruit (or pomelo), an orange and a tangerine. In the present study, antioxidant activity of rind extracts of *Citrus reticulate x Citrus paradise* was evaluated *in vitro* using DPPH, Nitric oxide, Hydrogen peroxide, Super oxide Dismutase free radical scavenging methods. [1] Different concentrations of ethanolic extracts showed radical scavenging activity of which DPPH assay showed an $IC_{50}$ value of about 18.9. [2-3]Thus this study suggests that *Citrus reticulate x Citrus paradise*is an effective plant in terms of antioxidant potential that can be exploited for development of plant based antioxidant formulations.

**Keywords:** Antioxidant, free radicals, *Citrus reticulate x Citrus paradise*, DPPH, nitric oxide, hydrogen peroxide, super oxide dismutase, scavenging ability.

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**P-21**

## SMART DEVICE FOR WATER PURIFICATION

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In today's world, sustainability, recycling & reusability is the necessity due to scarcity of resources. One such resource is water. Water is fundamental to all life forms, only 1/4$^{th}$ of it is available as fresh drinking water [1]. This resource is becoming scarcer in certain places, and its availability is a major concern. To accomplish this, there is a need of newer techniques/technologies that helps to eliminate industrial pollutants such as pesticide, paints and dyes and heavy metals.

The present work demonstrates a technology in the form of fabricated device with smart materials that eliminates wide contaminants from waste water.These materials are synthesized by free radical copolymerization reactions resulting into smart polymers. Smart polymers have an ability to dissolve in water at room temperature however when the temperature is increased above a specific point they precipitate. This property is attributed to the transformation of the polymers from hydrophilic to hydrophobic on increasing the temperature. The hydrophobic transformation makes these polymers to bean interesting contenders for adsorption of impurities in water. Ward *et al.* [2]. The polymers are outcome of two smart polymers (Temperature and pH) giving dual characteristics thus widening the scope of application. The fabricated unit is a synergistic combination of synthesized smart polymers with naturally occurring materials. This combination will aid in removing organic, inorganic and microbial impurities. Various industries evacuate waste water into drainage channels hence we have designed a prototype that is eco-friendly and cost effective, therefore may prove for better recycling in water purification systems.

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P-22

# STABILITY INDICATING HPTLC METHOD DEVELOPMENT AND VALIDATION FOR THE DETERMINATION OF ISRADIPINE IN PURE AND DOSAGE FORM

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**Abstract:**

**Objective:** A simple, specific, accurate, cost effective and precise and stability indicating HPTLC method was developed and validated for the determination of Isradipine in pure and doage form.
**Methods:** Baranda et al.[1], Gauhar R et al. [2], Benjamin H et al. [3] **:** Stability test were done through exposure of the analyte solution to Acid, Alkali, Oxidiative, Photo-degradation, Thermal degradation. The chromatographic separation was carried out using Camag Linomat V semi-Automated sample applicator with TLC Scanner III. Stationary Phase consisting of TLC plates (Merck) pre coated with silica gel 60F254 on Aluminum Sheets was used. Mobile phase comprising of Acetonitrile: Ethyl acetate: water (6:3:1 v/v/v).
**Results:** K.Anie Vijetha et al. [4], It is highly labile to alkaline and acid hydrolysis compared to oxidation. The correlation coefficient ($r^2$=0.9986) with slope and Intercept of 2875.3 and 344.43 respectively. The LOD and LOQ were found to be 0.0260 and 0.0788 respectively. The % RSD was found to be 1.510%. The percentage recovery was found to be 100.06%. Densitometric peak purity results indicated the absence of co-eluting peaks with the main peak of isradipine, which demonstrated the specificity of assay method
**Conclusion:** The proposed HPTLC method was validated and can be applied for the determination of isradipine in pharmaceutical formulations and used in routine laboratories.

**Key words:** Isradipine, HPTLC, ICH Guidelines, stability indicating, method development and Validation

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P-23

# GREEN CHEMISTRY: AN EFFICIENT APPROACH FOR THE SYNTHESIS OF SUBSTITUTED BENZIMIDAZOLE USING ALUMINA AS CATALYST

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**ABSTRACT:** Green chemistry is an area of chemistry andis frequently considered as a response to the need to reduce the damage of the environment by man-made materials and the processes used to produce them. The advantages of using this method are the formation of a mild, manipulable procedure which is ecofriendly avoiding hazardous solvents with a shorter reaction time and higher yield of the product.[1] Benzimidazole is a heterocyclic aromatic organic compound. It is an important pharmacophore and a favored structure in medicinal chemistry. Benzimidazole has a broad spectrum of biological activities and with a wide range of therapeutic properties like antibiotic, antibacterial, antifungal, antitumor, anti-inflammatory, anti-ulcer, antitubercular activities.Thus, we became interested in the study of synthesis of substituted benzimidazole by green synthesis techniques and furthermore to study their biological activities. In the conventional methods ofsynthesis the reactions need very long heating time, elaborate and the cost is higher and there are more chances of environmental pollution. The reaction rate of greener approach induced benzimidazole synthesis increases ten to hundred times and the yield of the product increases by 10-40% compared to that by the conventional methods. [2]Several green methods are available for the synthesis, but there is an equivalent importance for the development of various other effective protocols since the utilization of Benzimidazole derivatives is more not only in Pharmacy but also in various fields of chemistry. In this study substituted benzimidazoles are synthesized by exploiting green methods with alumina as a catalyst in acetonitrile under a premeditated experimental conditions. [3]

**KEYWORDS:** Benzimidazole, Green Chemistry, Alumina, Acetonitrile, O- Phenylenediamine

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3. A green synthesis of Benzimidazoles. D.Kathirvelan et al. Indian Journal of Chemistry. Vol 52B, pp 1152- 1156, 2013.

**P-24**

# DISCOVERY OF MULTI-TARGET INHIBITORS FOR HIF PROLYL HYDROXYLASES

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Hypoxia is a medical condition in which there is deficiency of oxygen in the body or specific tissues and is observed in conditions such as cerebral ischemia, ischemic heart disease and cancer. Living cells have an in-built salvation to combat the debilitating effects of hypoxia in the form of Hypoxia Inducible Factor (HIF1), a transcription factor that regulates the expression of genes involved in a plethora of functions including erythropoesis, angiogenesis and metabolism[1,2] . The expression of HIF1α subunit of this dimeric protein complex is regulated by a group of proteins referred to as HIF prolyl hyroxylases -1,2,3(PHD-1,2,3) in an oxygen dependent manner[3]. It had been discovered that inhibition of PHD was shown to have a neuroprotective effect in countering ischemia-induced neuronal damage *in vivo*[4].

The objective of our study is to identify inhibitors for PHD1 and PHD3 and in turn analyse their neuroprotective effect following ischemic stroke. Structures of PHD1 and PHD3 were derived using homology modeling and potential leads were identified by conducting virtual screening with FDA approved drug library. Further, molecular dynamics studies were performed to consolidate the protein-drug interactions.

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P-25

# Anticoagulant and cytotoxic activities of Novel Imidazolidine-2,4-dione, and 2-Thioxoimidazolidin-4-one Derivatives

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In this research, to investigated the synthesis and characterization of some imidazolidine-2,4-dione, 2-thioxoimidazolidin-4-one derivatives and synthesized compounds were evaluated for anticoagulant and cytotoxic activities. The synthesized compounds were confirmed by Fourier transform infrared spectroscopy (IR), proton nuclear magnetic resonance ($^{1}$H-NMR), carbon nuclear magnetic resonance ($^{13}$C-NMR), mass spectrometry (MS), and elemental analyses. The synthesized compounds were screened for MCF-7 breast cancer cell line and anti-coagulant activities. Anticoagulant activity was determined by activated partial thromboplastin time (APTT) and prothrombin time (PT) coagulation assays. Compound 3-(2,6-bis(4-methoxyphenyl)-1,3-dimethylpiperidin-4-ylideneamino)-2-thioxoimi dazolidin-4-one (>1000s in APTT assays ) was highly response in anticoagulant screening compared with the reference of heparin while the compound 3-{[-1,3-Dimethyl-2,6-di(4'-nitrophenyl)piperidin-4-ylidene]amino}imidazolidine -2,4-dione ($LD_{50}$: 20.4 µg/mL was highly active against MCF-7 breast cancer cell line compared with the reference. Therefore, the title compounds are novel and beneficial for the development of anticoagulant, and anticancer agents.

P-26

# FABRICATION OF COBALT FERRITE NANOPARTICLES FOR BIOMEDICAL APPLICATIONS

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**ABSTRACT:** Magnetic Nanoparticles have been widely investigated for their potential as mediators of heat for localised hyperthermia therapy. The cancer cells are highly sensitive to hyperthermia as compared to normal cells. The healthy cells can withstand upto 50ºC, in contrast the cancer cells undergoes apoptosis at 42ºC -45ºC. The Magnetic Nanoparticles has a good contrasting ability, hence have a wide applications in imaging and diagnostics. The Magnetic Nanocarriers have gained their importance in drug delivery since MNPs loaded with chemotherapeutic agent are physically targeted to the tumours and retained there by application of an external permanent magnetic field and thus undesirable side effects in healthy tissues are minimised. The objective of this study is to synthesize Cobalt ferrite magnetic nanoparticles for targeted drug delivery and hyperthermia applications. The Monodisperse cobalt ferrite nanoparticles were synthesized by Co-precipitation and Hydrothermal method. All the particles were structurally characterised by Scanning Electron Microscopy and X-ray Diffraction Pattern. The Magnetic behaviour of the cobalt ferrite is analysed using Vibrational Scanning Magnetometer.The fabricated cobalt ferrite can be used as a magnetic carrier for drug delivery with imaging and hyperthermia applications.

**P-27**

# Secretion of α-L-rhamnosidase from *Aspergillus* terreus MTCC – 3374 using solid state fermentation

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**Abstract:** α-L-rhamnosidases cleaves terminal α-L-rhamnose specifically from a number of natural glycosides (Wang, et al., 2015; Makino et al.,2009; Valentova, et al., 2014). The enzyme has wide occurrence in nature and is biotechnologically important (Rajal,et al,2009, Tamayo-Ramos & Orejas. (2014). Most of α-L-rhamnosidases reported so far have their pH optima in the acidic pH range. α-L-rhamnosidases with different physicochemical properties are suitable for different applications (Yadav et al., 2010). Therefore, there is a scientific need to identify different sources of α-L-rhamnosidases with different properties suitable for different applications. Here, we report a fungal α-L-rhamnosidases which have secreted by *Aspergillus terreus* MTCC- 3374 in solid state fermentation using corn cob, washed sugar cane bagasse, wheat bran, wheat straw, cotton, and polyurethane foam as substrate or support for the enzyme production. Cultures were carried out in the petri dishes under controlled humidity and temperature. Naringin and rhamnose were using the enzyme inducers and carbon sources. The enzyme activity was appreciably greater when using cotton or polyurethane foam than other solid support. The kinetic characteristics of these enzymes like $K_m$, pH and temperature optima using p-nitrophenyl- α-L-rhamnopyraniside as the substrate have been determined.

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**P-28**

## Synthesisof Nitrosobenzenesfrom arylaminesusing PlantPeroxidase

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**Abstract:** Enzymes being specific, efficient biocatalysts and operational under milder reaction conditions have great promise as future reagents in organic synthesis.[1,2] Corbett et al[3-5] have reported that chloroperoxidase from the marine fungus *Caldariomyces fumago* transforms 4–chloroaniline to 4–chloronitrosobenzene specifically in presence of $H_2O_2$. Recently we have purified chloroperoxidase from the juice of *Musa paradisiaca* stem and have demonstrated its classical peroxidase and halogenating activities.[6] In order to evaluate the potential of this plant chloroperoxidase in the transformation of arylamines to nitrosobenzenes, we have studied the substrate specificity of the chloroperoxidase of *Musa paradisiaca* stem juice for various substituted arylamines.

The enzymatic characteristics of *Musa paradisiaca* stem Chloroperoxidase using 4- chloroaniline as the substrate have been determined. The $K_m$ values for 4-chloroaniline and $H_2O_2$ were 770 µM and 154 µM respectively while the pH and temperature optima were 4.4 and $30^0$ C respectively. The substrate specificity of the enzyme for the substituted arylamines have been studied. The feasibility of the concentrated Musa paradisiacal stem juice for the specific conversion of 4- chloroaniline to 4-chloronitrosobenzene has been demonstrated.This communication reports a crude preparation of Chloroperoxidase from *Musa paradisiaca* which can be conveniently prepared and used for the transformation of aromatic amines to its nitrosobenzene. This is the first report of nitrosobenzene formation using a plant chloroperoxidase.

The method for the preparation of chloroperoxidase from the stem of *Musa paradisiaca* has been developed.

**Key words:** Peroxidase, Chloroperoxidase,N-oxidation, Metalloenzyme, Musa paradisiacal

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P-29

# A stability indicating UPLC method for simultaneous estimation of Emtricitabine, Tenofovir disoproxil fumarate and Efavirenz in pharmaceutical dosage form.

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**Abstract:** A simple, fast reproducible, reliable and sensitive UPLC method was developed for the simultaneous estimation of three anti-retroviral drugs in combination namely, Emtricitabine, Tenofovir disoproxil fumarate and Efavirenz. The chromatographic separation was carried out on a sub 2 micron particle size column Waters Acquity UPLC BEH C18, 100 x 2.1 mm, 1.7 µm to achieve more efficiency and better resolution in a gradient mode elution consisting of mobile phase A : Buffer (0.05% of Trifluro acetic acid in water) and mobile phase B: Methanol. Detection wavelength was set at 262 nm with a flow rate of 0.4ml/min.The retention times of Emtricitibine, Tenofovir disoproxil fumarate and Efavirenz was about 0.6, 1.88 and 3.23 minute respectively. Under optimized conditions all three components were well separated from each other and also from main degradation impurities like Monoester impurity of Tenofovir, S-Oxide impurity of Emtricitabine and Amino alcohol and Quinoline impurity of Efavirenz. This was further supported by forced degradation studies. The % RSD was well within the limits and the correlation coefficient was 0.999.

The developed method was validated as per ICH guidelines. Hence this validated method can be used in routine quality testing of individual dosage forms and combination.

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**P-30**

# Role Of GA Codon Box In Codon-Anticodon Pairing For The Two-Fold Degeneracy Of Aspartic Acid And Glutamic Acid

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Protein synthesis is a highly complex process which involves the conversion of the base/nucleotide sequence of DNA into the amino acid sequence of the protein synthesized. The protein synthetic machinery of the ribosome allows only cognate codon-anticodon pairs at the decoding site of the ribosome. The three bases of the mRNA i.e., codon are defined from the 5' to the 3' end, and likewise for the three bases of the anticodon of tRNA. Here we examine the role of wobble pairing of the GA Codon-Box with Guanine(G) and Queuosine(Q)/ 7-(3,4-*trans*-4,5-*cis*-dihydroxy-1-cyclopenten-3-ylaminomethyl)- 7-deazaguanosine anticodons coding for Aspartic Acid; 5-methyl-aminomethyl-2-thiouracil ($S^{mn}$) and Cytosine(C) coding for Glutamic Acid. In the Revised Wobble Rules, the $S^{mn}$ is proposed to wobble with Adenine and Guanine which codes for Glutamic Acid; whereas the Q has been studied to wobble with Uridine and Cytosine.The interaction between the codon and anticodon are studied using the force-field of AMBER which gives a better insight to the stability of these codon-anticodon system.The paper seeks to predict the trends to label any candidate wobble base pair as allowed or disallowed pairs on the basis of configurational markers to explain the two-fold codon degeneracy displayed by amino-acid Aspartic Acid and Glutamic Acid in the genetic code.

***Key Words*:** Codon-anticodon, cognate, *disallowed* wobble base pair

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P-31

# Nickel nano-particles, a reusable magnetic and efficient green catalyst for the synthesis of diverse heterocycles and their theoretical study

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**Abstract:** A library of diverse biologically important heterocycles was synthesized efficiently employing Ni nanoparticles. The protocol was developed via one pot multi-component reaction of barbituric acid/dimedone/4-hydoxy coumarin condensed with various substituted aldehydes in aqueous medium under room temperature catalysed by Ni nanoparticles a magnetically recyclable heterogeneous catalyst. The method is simple in its own way, facile and uses eco-friendly solvent giving excellent yield of the desired product without any column chromatographic method. The synthesised products were then theoretically studies using DFT calculations.

**Keywords:** Nanoparticles ; Green MCR; DFT calculations

P-32

# $SeO_2$-PTSA MEDIATED OXIDATIVE COUPLING OF ARYL METHYL KETONES WITH ALIPHATIC ALCOHOLS: AN EFFICIENT ONE-POT SYNTHESIS OF α-KETOACETALS

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*α*-ketoacetals (protected glyoxal derivatives) constitute a strategic array of functional groups of great value in synthetic organic chemistry. They offer the possibility of performing the selective functionalization of a keto group over the more reactive aldehyde, as the latter is protected as an acetal. *α*-ketoacetals are key intermediates in the preparation of chiral cyanohydrins, nicotine derivatives, chiral sulfoxides, α-hydroxy acetals, α-hydroxy esters, amino-alcohols, nitrogen and oxygen-containing heterocycles, chiral 1,2-diols. A new methodology for the synthesis of *α*-ketoacetals was developed through the oxidative coupling of aryl methyl ketones with aliphatic alcohols in the presence of selenium dioxide and para-toluenesulfonic acid. This method was found to be highly efficient, quite general and proceeded smoothly at ambient temperatures.

P-33

# Beta carboline analogues: A selective kinase inhibitors with unusual binding approach

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**ABSTRACT:** The development of potent and selective kinase inhibitors is a challenging task in modern drug discovery of anticancer drugs. The innate promiscuity of kinase inhibitors largely results from ATP-mimetic binding to the kinase hinge region. We present a novel class of 9-substituted-β-carbolines whose kinase inhibitory activity does not rely on canonical ATP-mimetic hinge interactions. A library of 200 carboline analogues were designed and their *in-silico* docking studies were performed towards PIM-1 (proviral integration site in Moloney murine leukemia virus; PDB id-3CY2) by GLIDE integrated Maestro 9.9. The docking results show an unexpected inverted binding mode of our designed compounds with PIM1. The presence of halogen bonds impart a major role for binding with kinase backbone residues on oncogenic PIM1. All the designed compounds exhibited good binding interactions with the active site residues. Therefore, we suggest that this scaffold may serve as a valuable template for the design and development of specific inhibitors of PIM1 kinase proteins.

**KEYWORDS:** Carbolines, Cancer, PIM-1, Docking, Kinase inhibitor.

P-34

# DESIGN, SYNTHESIS, CHARACTERIZATION AND CYTOTOXIC STUDY OF 3-METHYL-2-OXO-*2H*-CHROMEN-7-YL STEARATE

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**Abstract:** As estrogens are well known to play crucial roles in breast cancer development, much effort has been devoted to block estrogen formation. Although the current existing drugs used for the treatment of breast cancer function as an anti-estrogen in the breast, they also function as an estrogen receptor agonist in the uterus and elevates a woman's risk of getting uterine cancer. This would be due to the lack of selective binding and partial agonistic effect of the existing drugs towards the estrogen receptors. Coumarin and its analogues have shown remarkable activity against breast cancer cell lines through inhibition against estrogen receptors. The extension of side chain length of the coumarin nucleus at 3rd and 7th position has shown to increase the receptor binding affinity. It has been proved that poly unsaturated fatty acids have beneficial effects in chemotherapy. Keeping in mind the estrogenic receptor inhibitory properties of coumarin nucleus and anti-breast cancer activity of fatty acids, it is proposed to design and develop novel pharmacophores containing coumarin and fatty acid scaffold. *In-silico* docking studies have been carried out in to the crystal structure of human estrogen receptor [PDB id 2IOG].Totally eighteen compounds which showed good docking results have been taken for further synthesis. Among them, one of the compound 3-methyl-2-oxo-*2h*-chromen-7-yl stearate has been synthesized and characterized by spectral analysis. The compound has been screened for its anti-breast cancer activity against MCF-7 cell lines by MTT method and the results are compared with standard tamoxifen. The synthesized compound has shown good CTC50 values than tamoxifen.

**Key words:** Breast cancer, Fatty acids, Coumarin

P-35

# PHARMACIST ROLE IN CONTROLLING NEGLECTED DISEASES – AN ESSENTIAL DISCUSSION TO CALL FOR A COLLABORATIVE WORK

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**ABSTRACT:** One of the objectives of the World Health Organization (WHO)is to ensure "effectiveco-ordination and support provided to WHO Member Statesin order to provide access for all populations to interventionsfor the prevention, control, elimination and eradication ofneglected tropical diseases, including zoonotic diseases"[1]. Many documents highlight the devastating impactsof neglected tropical diseases (NTDs) on human health andthe socioeconomic development of many impoverishedcommunities. A growing body of evidence demonstrates thatcontrol of these diseases will significantly reduce illness, socialexclusion and mortality [2]. Furthermore, prevention and controlof NTDs will contribute directly to the attainment of severalMillennium Development Goals. Globalization has increased the awareness of global health disparities, helped to decrease global disease burden and increased global health education demand, often addressed by academic global health programs of high income nations in low to middle income nations [3,4]. Pharmacists can make a unique contribution to the outcome of drug therapy, to their patients' quality of life and to public health. Pharmacists have a critical role to play and a gap to fill in the health workforce.Pharmacistscan primarily work to explore and identify examples of key pharmaceutical-related public health problems in India, and secondly, to introduce and evaluate student interest in global health pharmaceutical issues, activities and potential careers. The incorporation of global health policy into pharmacy curricula illustrate examples of higher education contributing to shaping future health professional roles and career interests for new and expanding service opportunities in the global health workforce. The implementation and practice of pharmaceutical care must be supported and improved by measuring, assessing and improving pharmacy practice activities, utilizing the conceptual framework of continuous quality improvement.

**Key words:** Global health, neglected diseases, millennium development goals, pharmacist role

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**P-36**

# Appraisal of hydro alcoholic fruit extract of *Citrulluscolocynthis* in Type II collagen induced arthritis mediated diabetes in Rats

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**ABSTRACT:**

**Aim:** To evaluate the hydro alcoholic extract of *Citrullunscolocynthis* on arthritis mediated diabetes in Rats

**Methods:** Type II collagen in FCA was used to induce the arthritis to the animals. 0.2mlemulsion was injected into the intra dermal of tail on 0 day. Booster injection was given to the animal on 7th day. Animals were kept for 14 days for development of arthritis. Treatment was started 14th day to 28th day. Blood samples, joints and pancreas was isolated for the examination at end of the study.

**Result:** TNF-α and IL-6 in RA appear to block the function of insulin at the receptor level[6], also dysfunction of β-cells.[1,2]TNF-α, IL-6, RF, and blood glucose levels were significantly reduced in drug treated group. The present result showed statistically significant result and the histopathology of joints and pancreas in drug treated group further strength then the efficacy of this plant against inflammation induced diabetes.

**Conclusion:** From the result, it can be concluded that the hydro alcoholic extract of *C.colocynthis* fruit possess anti-arthritic activity and it inhibited the inflammation mediated diabetes mellitus.

**Key words:** *Citrulluscolocynthis*¸TNF-α, IL-6, RF.

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**P-37**

# Lipid delivery of NMITLI118RT+: A promising therapy for ischemia induced neuro-degeneration

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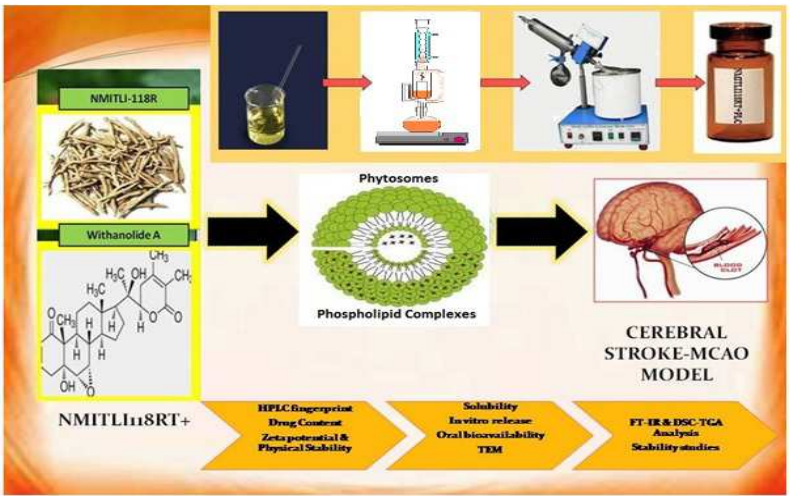
**Abstract:** NMITLI118RT+ (a standardized ethanolic root extract of a new chemotype of *Withania somnifera* L.) developed by CSIR, India is a potential lead for the management of cerebral stroke. The authors investigated its beneficial effects in ischemia induced neuro-degeneration. Lipoidal delivery system of NMITLI118RT+ was envisaged for its efficient delivery. The developed formulation was pharmaceutically characterized and evaluated for its neuro-protective potential against experimenal stroke in rat MCAO model. Characterization studies included solubility studies, dissolution profile, compatibility studies (based on FT-IR and DSC-TGA analysis), zeta potential, physical stability, stress induced degradation and photostability studies. Findings revealed the beneficial effects of NMITLI118RT+ could be augmented by its formulation in 1 hour pre and 6 hour post treatment as was evident from reduction in MDA levels, increment in GSH levels, reduction in neurological deficit scores and reduction in infarct size. The study could demonstrate favorable outcomes of NMITLI118RT+ via lipid delivery in brain function restoration following stroke.

**Keywords:** *Withania somnifera*, phytosomes, stroke, ischemia, phospholipid complexes.

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P-38

# Synthesis and Antimicrobial Activity of Some Phenothiazole Metal Complexes of Chalcones

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**ABSTRACT:** Now a day there is a great interest in synthesis and characterization of Chalcone ligands which contains O, N, S sequence and their metal complexes. Chalcones derived from Aromatic ketones and aromatic aldehydes have a wide variety of applications in many fields, *e.g.*, biological, inorganic and analytical chemistry.

Chalcones were tested for antimicrobial activity, which is related to their chemical structure. Metal complexes of chalcones are extensively studied due to synthetic flexibility, selectivity and sensitivity towards a variety of metal atoms. They are found useful in catalysis, in medicine as antibiotics and anti-inflammatory agents. These metal complexes have found extensive application in various fields of human interest.

Chalcones of substituted phenothiazole with 4-chlorobenzaldehydes and their Transition metal complexes have been synthesized. The synthesized chalcones and the corresponding complexes have been characterized by spectral analysis viz IR, $^{1}$H NMR, Electronic, XRD, solution conductivity and their Magnetic moment. The spectral studies indicate octahedral geometry for Co (II), Ni (II) and Fe (II) complexes and tetrahedral geometry for the Zn (II) and Mn (II) complexes. From XRD study, monoclinic, 'p' type crystal structure can be assigned to the synthesized complexes. The complexes were also screened for antifungal and antibacterial activities. The antimicrobial screening shows that the metal complexes show the enhanced activity than their corresponding ligands.

P-39

# Highly selective, Metal free hydroxylation of 2-arylidene indane-1,3diones With Isocyanide for the Construction of quaternary Carbon Center *via* Michael addation reaction

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Firstly reported solvent containing water as an -OH source for highly selective, novel catalyst metal free hydroxylation of **2-arylideneindane- 1,3 indanediones** for the construction of quaternary carbon centerC-C and C-O bond formation by isocynide promoted Michael addition reaction.

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**P-40**

# A multicomponent reaction approach towards the synthesis of novel indole-curcumine hybrids as potential antidyslipidemic agents

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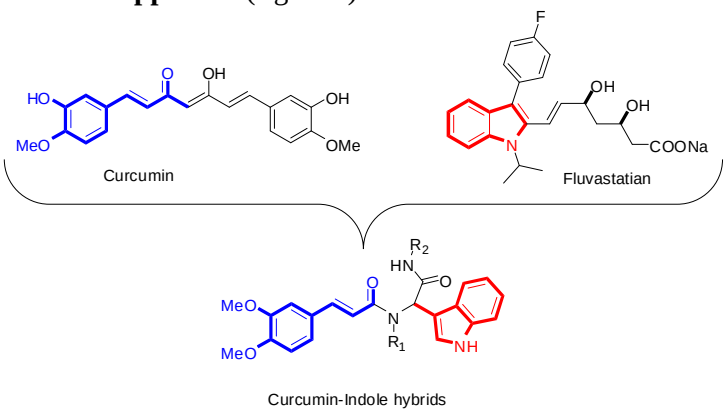
Today in most of the developed and developing countries, hyperlipidemia and thereby atherosclerosis is the leading cause of cardiac illness and deaths.[1] Hyperlipidemia is a major cause of atherosclerosis and atherosclerosis-associated conditions such as coronary heart disease, ischemic cerebrovascular disease, and peripheral vascular disease. Fibrate class (PPARa agonists) of drugs, which are mostly used to treat hyper triglyceridemia and low HDL-cholesterol, requires high doses to show significant efficacy.[2]In addition, a combination of fibrate and statins has met with serious safety concerns as exemplified by the withdrawal of Cerivastatin in 2001. Therefore, there is a constant need for a different class of potent compounds to treat dyslipidemia without severe side effects.In the continuation of our ongoing programme to develop new hybrid molecules[3], and inspired bythe biological importance of curcumin and indole based natural product, Herein, we wish to describe the synthesis and antidyslipidemic evaluation of novel curcumin-indole based hybrids *via***multicomponent reaction approach** (figure 1)

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P-41

# Novel Fibrinolytic activity of partially purified Exopolysaccharides (EPSs) of marine bacterium *Terribacillus saccharophilus*

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Marine environment has gained attention as it serves a source of novel bioactive compounds. Exopolysaccharides (EPSs) is one of the important bioactive compound produced by marine bacteria. Marine bacteria produced EPSs in response to biotic like competition and to abiotic such as temperature, light intensity, pH, salinity etc stress factors as strategies of adaptation to extreme environments. The physiological role of EPSs depends on the habitat and the natural conditions in which bacteria live. Present work is mainly focused on marine EPSs producing bacterium PS-47 isolated from Bhavnagar coast, Gujarat, India. *Terribacillus saccharophilus* produced copious amount of EPSs i.e, 1052 µg/ml in unoptimized conditions. EPSs had been partially purified by using alcohol and TCA. The EPSs exhibited fibrinolytic activity in which lysis of plasma clots was observed using to pentosan sulphuric polyester as a standard. These EPSs with promising fibrinolytic activity would be applicable in pharmaceutical industry. Further research will be carried out to elucidate the structure and chemical composition of the produced EPSs and other possible biotechnological potential.

**Key words:** Marine bacteria, Exopolysaccharides (EPS), fibrinolytic activity

**P-42**

# Ionic liquid catalyzed Synthesis of 1,4 benzoxazepinone and 1,4 benzodiazepinone Analogues via Sequential Ugi post Intramolecular cyclization

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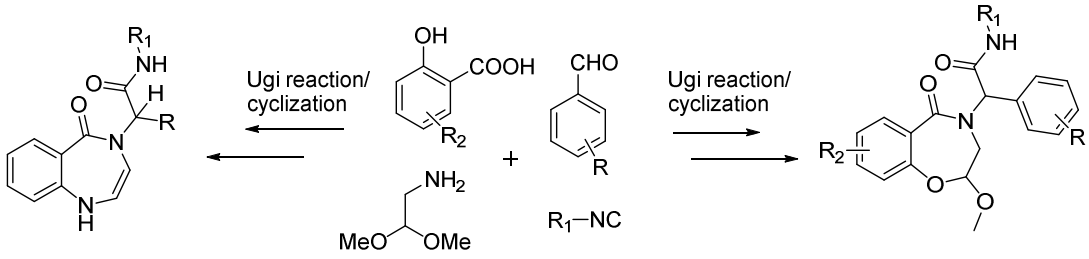
**Abstract:** Benzofused heterocyclic, 1,4 benzoxazepinone and 1,4 benzodiazepinone are one of the prominent class of privileged scaffold gained important significance in Medicinal chemistry for construction of bioactive natural products, drugs and therapeutic leads. 1,4 benzoxazepinone and 1,4 benzodiazepinone known for wide spectrum of biological activities like psychotropic, neurotropic, anti-inflammatory, anticonvulsants, HIV-1 reverse transcriptase inhibitor, antitumor agent, antithrombotic, antiepileptic, progesterone agonist, antifungal, analgesic, anxiolytics, antihistaminic, anti aggregating, epidermal growth factor receptor (EGFR) tyrosine kinase inhibitory acti vities.[1]
Ionic liquids (ILs) have been widely used as an environmentally acceptable reaction medium or catalyst in green synthesis over the past decade owing to their advantages of nonvolatility, thermal stability, recyclability, and tunable chemistry.[2]

In the light of above fact, herein we report an efficient two step process for the synthesis of 1,4 benzoxazepinone analogus has been developed. This protocol involves the Ugi four-component reaction (U-4CR) followed by an intramolecular ionic liquid catalysed cyclization of the Ugi intermediate to afford the desired products in good to excellent yields. In addition, we synthesized 1,4 benzodiazepinone derivatives of medicinal importance using Ugi product followed by intramolecular cyclization.

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**P-43**

# Recyclable Pd(II)complex catalysed oxidative $sp^2$ C-H bond acylation of 2-aryl pyridines

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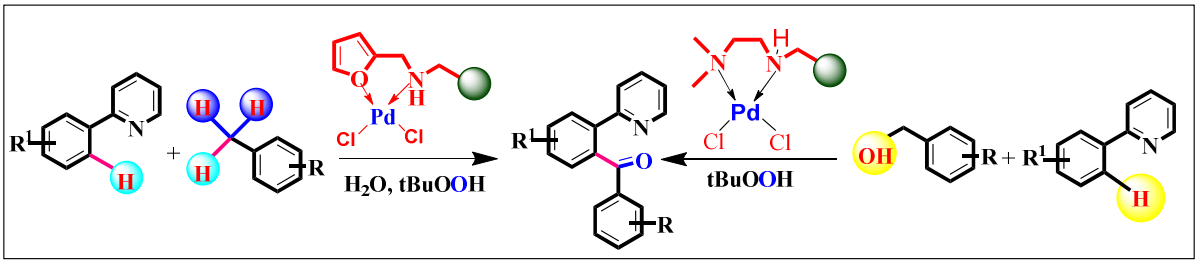
**Abstract**: Design and development of direct aromatic C–H bond functionalization is one of the most challenging that has gained considerable attention over traditional cross-coupling methods [1]. Benzophenones constitute prominent structural motifs of top 200 most-sold pharmaceuticals that exhibit broad spectrum of biological activities [2]. In view of minimizing the waste/side product formation for acylation bearing ortho-directing group [3,4], we have developed a simple polystyrene supported Pd(II) catalysts.This polystyrene-supported Pd(II) complex was used as an efficient catalysts for synthesis of aromatic ketones *via ortho*-acylation of $sp^2$ C-H bond of 2-aryl pyridines with toluene and alcohols as an effective coupling partner. The alcohols and toluene derivatives were oxidized with TBHP to their corresponding aldehydes *in situ* and efficiently coupled with 2-aryl pyridines to form aryl ketones under mild conditions. Furthermore, the catalyst could be easily recovered by simple filtration and reused for five cycles without any significant decrease in its activity.

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**P-44**

## Mechanism of cationic antimicrobial peptide Pellino-1 from a crustacean

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In recent years, the rapid evolution of pathogenic bacteria has been a greater challenge for pharmaceutical companies for the development of antibiotic drugs. Among the different approches to fight against the pathogenic invasion, the antimicrobial peptides are considered as new generation of antibiotic drugs. The remarkable functions of cationic antimicrobial peptides have obtained a significant place in clinical and preclinical studies. The identified cationic peptide was determined with potent bactericidal activity against ten pathogenic bacteria without showing any significant cytotoxicity to the HEK293 cell lines and also against the human erythrocytes. Further investigations with flow cytometric analysis and SEM imaging revealed that the peptide has the ability to permeabilize the bacterial membrane of *Bacillus cereus* ATCC 2106. Interestingly, along with membrane disruption the peptide *Mr*DN also prominently binds with the bacterial DNA, which resulted in a differential electrophoretic migration. From this study, a potential antimicrobial peptide, *Mr*DN was determined to have a broad range of antimicrobial activity and its mechanism of action also determined by using *Bacillus cereus* ATCC 2106 model.

**P-45**

# Pd-$Fe_3O_4$/NrGO Catalyzed Cascade Isocyanide Insertion Reaction under Mild Condition

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Substituted quinazolinones are ubiquitous structural motifs of many natural and synthetic biologically active compounds. A ligand-free Pd-$Fe_3O_4$ supported on N-doped reduced grapheme oxide (N-rGO) catalyzed isocyanide insertion reaction has been found to occur between wide range of aryl iodides/amines and ortho-functionalized aromatic isocyanides for the synthesis of biologically relevant quinazolinones under extremely mild condition.[1] The catalysts were characterized by means of spectroscopy (FT-IR, XPS, AES), surface area analysis (BET), and transmission electron microscopy (TEM). HR-TEM shows that the catalytic nanoparticles are reasonably dispersed with no agglomeration (Figure 2a). Ordered crystalline structure of N-rGO supporter was demonstrated by interlayer distance 0.37 nm of restored graphitic layers (Figure 2c). The atomic scale image by STEM with a probe correction and ~0.1 nm point resolution provided the evidence for close proximity between the Pd and the $Fe_3O_4$ particles. The brighter part (yellow circle) corresponds to Pd atoms (Figure 2b) and the less bright part to Fe atoms (Figure 2b) because the intensity is directly proportional to the square of the atomic number of the elements. Besides, this is the first general magnetically separable N-doped graphene-supported heterogeneous catalyst for isocyanide insertion reactions with excellent recyclability.

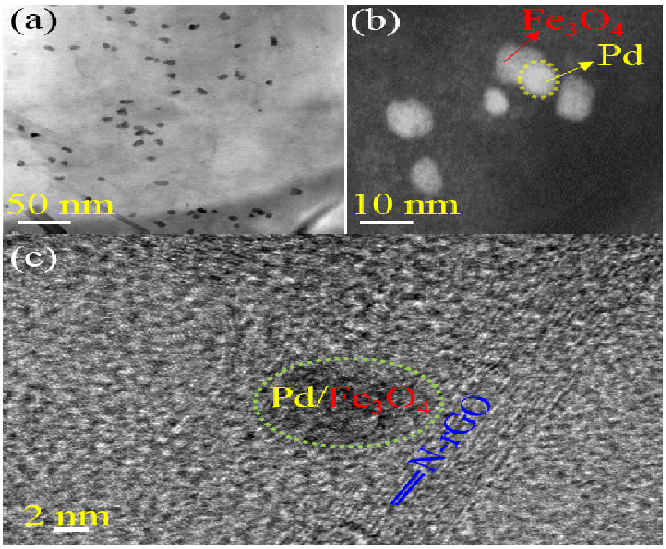


**Figure 1. TEM image of Pd-$Fe_3O_4$/NrGO.**

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**P-46**

## Nonestrogenic Bone Conserving Effect of Medicarpin in Ovariectomized Mice

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Medicarpin, a natural compound shows chemical similarity with isoflavonoids, is found in a wide range of leguminous species including chickpea and in the extracts of *Butea monosperma*.[1] Medicarpin, a pterocarpan class of naturally occurring oxygen heterocyclic compound was synthesized in gram scale to investigate its effects on murine bone cells and in ovariectomized (OVx) mice. Medicarpin, at as low as $10^{-10}$ M suppressed osteoclastogenesis in bone marrow cells (BMCs). Medicarpin induced apoptosis of mature osteoclasts isolated from long bones.[2-3]

The study was conducted in accordance with current legislation on animal experiments [Institutional Animal Ethical Committee (IAEC) at C.D.R.I.]. Eight week old adult female Balb/c mice were used for the study. Animals were housed at 21 °C, in 12-h light: 12-h dark cycles. Normal chow diet and water were provided *ad libitum*. Ten mice /group were taken for the study and the groups were as follows: sham (ovary intact) + vehicle (gum acacia in distilled water), Ovx + vehicle, Ovx + 1.0 or 10 mg.kg-1 body weight dose of medicarpin. Mice 259 were treated with 1.0 and 10.0 mg.kg-1 body weight dose of medicarpin or vehicle once daily for 4 weeks by oral gavage. After the period of four weeks animals were sacrificed and femur bones were collected for analysis of trabecular microarchitecture.[4]

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**P-47**

# Synthesis of *N*-substituted 4-aminoquinoline-pyrimidine molecular hybrids and their antimalarial activity, heme binding and docking studies

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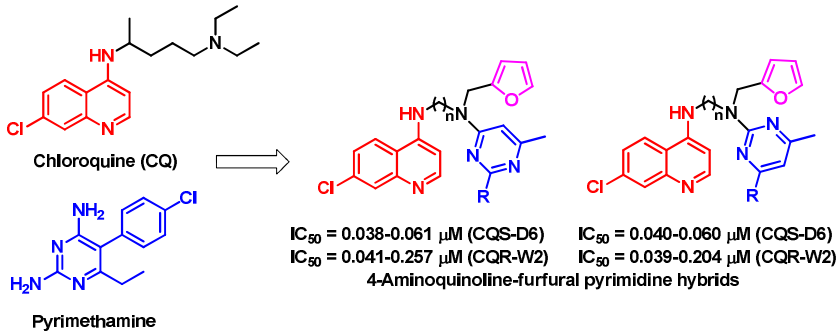
**Abstract:** Malaria is one of the world's greatest global public health challenges [1]. The traditional first line antimalarial drugs belonging to the 4-aminoquinoline class have been used for the treatment of malaria for a long time but *P. falcifarum* has developed resistance against these compounds [2]. In order to overcome the resistance problem, molecular hybridization has proven to be a promising tool [3-5]. In this regard, we have synthesized a series of novel *N*-substituted 4-aminoquinoline-pyrimidine hybrids *via* simple and economic route and evaluated for their antimalarial activity. Most of the compounds showed potent antimalarial activity against both CQ-sensitive and CQ-resistant strains with high selectivity index. The compounds were found to be non-toxic to the mammalian cell lines. The most active compound was analysed for heme binding activity using UV-spectrophotometer. Compound was found to interact with heme and a complex formation between compound and heme in a 1:1 stoichiometry ratio was determined using Jobs' plot. The interaction of these hybrids was also investigated by the molecular docking studies in the binding site of wild type *Pf*-DHFR-TS and quadruple mutant *Pf*-DHFR-TS. The pharmacokinetic property analysis of best active compounds was also studied by ADMET prediction.

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**P-48**

# Synthesis and biological evaluation of hydroxytriazenes as anti-radical and anti-diabetic agents

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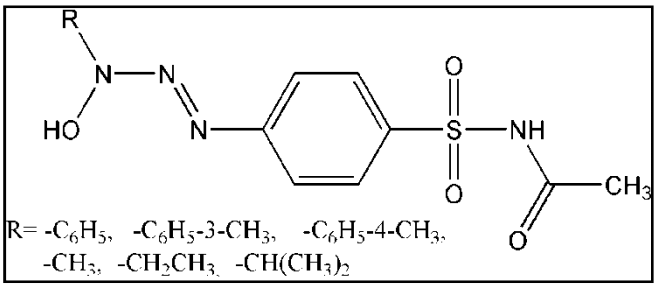
**Abstract:** Hydroxytriazenes are well established chelating agents[1] and show broad spectrum of biological activities[2]. These compounds are synthesized by aryl diazo coupling reaction with hydroxyl amines. In the present presentation, six hydroxytriazenes were synthesized by N-[(4-aminophenyl)sulfonyl]acetamide moiety with different nitro derivatives and anti-radical and anti-diabetic activities of hydroxytriazene derivatives were evaluated by DPPH scavenging[3] and α-glucosidase inhibition method[4] respectively. Among the tested compounds I, III and IV showed significant anti-radical activity at 0.01–0.05 mg/mL concentration and compound V and IV showed good anti-diabetic activity with $IC_{50}$ values 0.225 and 0.277 mg/mL respectively. The study highlights potential activity of this series of hydroxytriazenes[5].




**Key Words:** Hydroxytriazene, anti-radical and anti-diabetic agent

**Reference:**

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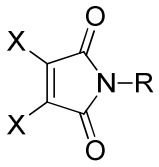
P-49

# Synthesis of novel *N*-substituted maleimide derivatives as spermicidal agents

Suyash Pant, Dr. V.L. Sharma

**Abstract:** Birth control, also known as contraception and fertility control, includes methods or devices used to prevent pregnancy.[1] Birth control methods have been used since ancient times, but effective and safe methods only became available in the 20th century. Spermicidal agent has the ability to immoblize 100% human spermatozoa[2] immediately after ejaculation at physiological condition. Women controlled spermicidal microbicide offer a suitable alternative to condom and provide protection from STIs and unwanted pregnancy.[3] Maleimide and *N*-alkyl maleimide derivatives are known to be thiol inhibitor and has the potential to immoblize sperm. Further to explore this maleimide scaffold, it was planned to synthesize some novel maleimide and 3,4-maleimide derivatives (Fig 1). Based on the literature reports and the ability of bromomaleimides to react with thiols present over proteins, these novel series of bromo maleimide derivatives may have the ability to immobilize sperm. In this view a series of compounds would be synthesized and subjected for their spermicidal activity and the most active compound of the series would also evaluated for *in vivo* activity also.




X= SR, Br
R= aralkyl

**Fig 1.** maleimide and 3,4-maleimide derivatives

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**P-50**

## In search of small molecule Glucagon like peptide-1 receptor (GLP-1R) agonist

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**Abstract:** Glucagon-like peptide-1 receptor (GLP-1R)is a very attractive target for treatment of Type 2 diabetes[1]. The clinical effectiveness of GLP-1 mimetics to improve glucose control in patients strongly supports discovery pursuits aimed at identifying and developing orally active, small molecule GLP-1R agonists. The discovery of orally active small molecule agonists has been generally unsuccessful[2]. In the present work, we have used homology model of GLP-1R to explore and validate the putative site for quinoxaline analogs[3] through SBDD approach. The GLP-1R homology model was further subjected to 500ns molecular dynamics simulation and studied various structural snapshots to identify the structure of GLP-1R showing best correlation between $pEC_{50}$ and various scores (docking score, MM-GBSA ΔG bind, and WM/MM ΔG bind). Excellent correlation**($R^2$ =0.94)** between $pEC_{50}$ andWM/MM ΔG bind for the structural snapshot taken at 350ns was observed after induced-fit docking with most potent molecule of the series. This model was further used for virtual screening to predict potential small molecule agonists against GLP-1R.

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**P-51**

# Synthesis and cytotoxicity evaluation of condensed thienopyrimdines derivatives as ruatecarpine analogues

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**Abstract:** Rutaecarpine is a pentacyclic indolopyridoquinazolinone alkaloid found in *Evodia rutaecarpa* and other related herbs. It has a variety of intriguing biological properties, which continue to attract the academic and industrial interest. Our interest was mainly focused on condensed thienopyrimidines due to its wide range of biological activity. We have reported thieno(2,3-*d*)pyrimidine derivatives as antihyperlipidemic and Gefitinib analogues . Very recently we have identified condensed thieno(2,3-*d*)pyrimidine derivatives as bioisosteres of rutaecarpine possessing antihypertensive activity. We found structural similarities between our reported test compounds with evodiamine and ruatecarpine. Twenty derivatives were synthesised by Niementowski condensations from anthranilic acids. An efficient procedure for preparation of the substituted thienopyrimidines has been established by the reaction of lactam salts with $POCl_3$ followed by amino acids, a displacement/amino ester cyclization takes place. The synthesized derivatives were evaluated for their in vitro cytotoxicity.

**Keywords:** Condensed thienopyrimidines, cytotoxicity, ruatecarpine

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**P-52**

# STRUCTURE BASED DRUG DESIGN OF PPARY AGONISTS PROVING EFFICACY FOR DIABETES AND CARDIOVASCULAR DISEASE

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Cardiovascular disease is the most common cause of morbidity and mortality among patients with Type II diabetes mellitus (T2DM). Peroxisome proliferation-activated receptor gamma (PPARY) is a nuclear receptor regulating transcription of several genes involved mainly in fatty acid and energy metabolism. PPARY agonists are used as insulin sensitizers for treatment of diabetes. Structure based drug design of Thiazolidinedione (glitazones) as ligand and PPARY as the receptor provided ligand interactions with receptor protein. Molecular level interactions between protein target and developed ligands maneuvered to design new molecules with improved protein fitting. The structured based design of Thiazolidinedione derivatives for PPARY agonist would serve as a benchmark for alteration of existing ligands to design new ones with better binding interactions.

**Keywords:** Diabetes Mellitus, PPARY, Thiazolidinedione, Drug Design.

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P-53

# HEPATOPROTECTIVE AND ANTIOXIDANT ACTIVITY OF *COCCINIA GRANDIS* ROOT EXTRACT AGAINST PARACETAMOL INDUCED HEPATIC OXIDATIVE STRESS IN WISTAR ALBINO RATS

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**ABSTRACT:**

Objective: To evaluate the Hepatoprorective and antioxidant activity of *Coccinia grandis* root extract against Paracetamol induced hepatic oxidative stress in Wistar albino rats.

Methods: Hepatoprotective activity of the ethanolic extract was evaluated for serum SGOT, SGPT, SALP, Total Bilirubin and Protein levels at two different dose level (200mg/kg and 400 mg/kg) in Paracetamol induced liver damaged Wister albino rats. Manokaran et al [1].

The antioxidant potential of the ethanolic extract of *Coccinia grandis* root was examined for enzymatic antioxidant activity, using SOD, CAT, Px, and GPx, and non-enzymatic antioxidant Reduced glutathione (GSH). Vadivu *et al.*[2,3]. The hepatoprotective and antioxidant activity were produced by ethanolic extract of *Coccinia grandis* with the std drug silymarin(25mg/kg).

Results: The standard drug Silymarin treated group showed significant ($P<0.01$) result compared to Paracetamol treated control group. The ethanolic extract of *Coccinia grandis* root produced significant ($P<0.01$) Hepatoprotective activity by reducing the elevated levels of SGOT, SGPT, SALP and elevated the decrease levels of Total Bilirubin and Protein at 200mg/kg dose. The standard drug Silymarin treated group showed significant ($P<0.01$) result compared to Paracetamol treated control group. The decreased levels of antioxidants SOD, CAT, GPx activities were reduced significantly ($P<0.01$) by ethanolic extract of *Coccinia grandis* at 200mg/kg dose level. The results were comparable with that of std drug silymarin 25mg/kg in paracetamol induced hepatotoxic rats. The hepatoprotective activity produced by ethanolic of *Coccinia grandis*(400mg/kg) was comparable with the hepatoprotective activity produced by std drug silymarin.

Conclusion: The ethanolic extract of roots of *Coccinia grandis* exhibits Hepatoprotective as well as antioxidant activities.

**Keywords:** *Coccinia grandis* root, ethanol, Paracetamol, Hepatoprotective & Antioxidant.

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**P-54**

# Highly efficient and regioselective synthesis of spirooxindolo pyrrolizidines by reaction of isatin, proline and acrylonitrile/methyl acrylate in water

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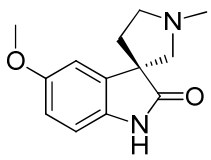
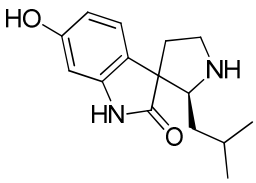
The synthesis of drug-like spirocyclic compounds has attracted considerable attention due to their wide spread applicability in biomedical sciences as they show great potential for binding to many biomolecules.[1] In particular, the spirooxindolo pyrrolidine kind of framework constitutes the core units of many naturally occurring alkaloids such as horsfiline,[2,3] elacomine[4] and mitraphylline.[5] Recently, these kinds of molecules have been shown to possess promising antitubercular activity.[6]

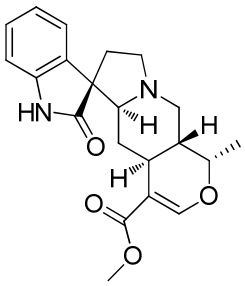
A simple, ecofriendly and regioselective three-component condensation of nonstabilzed azomethine ylides generated in situ from isatins and L-proline with acrylonitrile/methyl acrylate to give spirooxindolo pyrrolizidines has been realized. The reaction highlights the use of water as a reaction medium with good to excellent yields of products from readily available precursors.[7]




Horsfiline




Elacomine




Mitraphylline

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P-55

# Microwave induced Chemical Modifications of Sesquiterpene Lactones and to evaluate them in terms of PGR's and Lipid Peroxidation bioassays

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**ABSTRACT:** Sesquiterpene lactones having α – methylene –γ – lactone moiety have been established as potent plant growth regulators. With a view to increase the water solubility of lactones, diethanolamine adducts of parthenin (isolated from *Partheniumhysterophorus*) ,isoalantolactone&alantolactone (isolated from *Inularacemosa* ) were prepared. In order to introduce diethanolamine group in epoxyalantolides , isoalantolactone&alantolactone were allowed to react with an excess of perbenzoic acid followed by diethanolamine. In order to prepare more compounds for biological screening, diethanolamine was treated with isotelekin and isotelekin acetate. A further enhancement in rection rate was observed when reaction was done 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 biological evaluation as plant growth regulators and tested for their toxicological behaviour . The parameters studied in biological activity include adventitious root formation in hypocotyl cuttings of *Vignaradiata, Cucumismelo* cotyledon expansion test and seed germination studies in *Triticumaestivum.* 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.

**Key Words:** *Saussurealappa, Inularacemosa,* Compositae, sesquiterpene lactones, microwave irradiation, diethanolamine.

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P-56

# GENOTOXIC STUDY OF ARSENIC ON CHROMOSOMAL STRUCTURE OF MICE

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**ABSTRACT:** Arsenic (As) is a toxic metalloid element that is present in air, water and soil. Inorganic arsenic tends to be more toxic than organic arsenic. The incidence of arsenic contamination of ground water used for both irrigation as well as for human consumption or industrial activities has taken the dimension of an epidemiological problem. It has been established that inorganic arsenic is extremely toxic when administerd acutly and chronically. The present study is designed to study the genotoxic effects of arsenic on structure of chromosome in swiss albino mice. Albino mice were divided into three groups. Group I were kept as control. Group II were administrated an oral dose of arsenic trioxide 5mg/kg b.w. for 15 days. Group III were given an oral dose of arsenic trioxide 5mg/kg b.w.for 45 days.The autopsies were done from all the groups at 15 and 45 days post-treatment and bone marrow was removed for chromosomal study. It is concluded from the study that long term arsenic exposure causes chromosomal anomalies through heterogenous structure, elongation which leads to fragmentation of chromosomes.

**Key Words:** Arsenic (As), Heterogenous and Chromosomes

P-57

# Design, synthesis and characterizations of some new series of π-electron deficient poly-substituted thiouracil derivatives for their antifungal activity

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Nitrogen heterocycles possess a wide range of pharmacological activities and play a significant role in medicinal chemistry. Due to development of drug resistant parasites in parasitic area, the currently available drugs are not effective because of their limited pharmacological efficacy. Hence, the development of drug resistant parasitic strain has emerged as major challenge to the researchers to search new effective therapeutic agents for the treatment of patients suffering from drug resistant parasites. Keeping in view importance of the search of the new leads for the development of potential therapeutic agents [1] and continuation of our work on the synthesis of new heterocycles lead for their pharmacological activity [2,3], we envisioned our approach toward the synthesis of some new series of π-electron deficient poly-substituted thiouracil derivatives for their antifungal activity. In this presentation, the detailed synthetic procedure, characterizations of the synthesized compounds by their spectral data analysis and antifungal activity profiles will be discussed.

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**P-58**

# EFFECT OF FLY ASH ON EARTHWORM, *EISENIA FETIDA*

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**ABSTRACT:** Fly ash is receiving alarming attention due to its hazardous nature, widespread usage, and the manner of disposal, leading to environmental deterioration. Fly ash is a serious source of air pollution since it remains air borne for a long period of time and causes health hazards. Besides being a health hazard, fly ash degrades the environment. The conventional disposal method for fly ash leads to degradation of arable land and contamination of ground water. This work is carried to study the risk assessment of fly ash in earthworms as a model system. Earthworms were allowed to grow in fly ash. Biochemical studies were carried out to know the content of protein, cholestrol and glycogen in earthworm, *Eisenia fetida* on 0, 15 and 30 day of exposure to fly ash. The body weight of the worms and biochemical contents like cholestrol and glycogen were significantly increased on 15 day and 30 day exposure. The protein content in earthworms was significantly reduced on 15 day and 30 day exposure. The results of the present study show that fly ash has adverse effects on *Eisenia fetida*.

**Keywords**: Fly ash, *Eisenia fetida* and Chemical composition.

P-59

# Synthesis, characterization and *in-vitro* antioxidant study of hybrid urea/thiourea derivatives

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**Abstract:** A series of urea/thiourea derivatives were synthesized and their structures were confirmed by different spectroscopic method ($^{1}$HNMR, Mass, FT-IR) [1]. The *in-vitro* antioxidant potential of newly synthesized hybrid urea/thiourea derivatives were carried out by different antioxidant assays such as DPPH free radical scavenging, super oxide anion radical scavenging, nitric oxide scavenging and lipid peroxidation [2]. The compounds exhibited potent DPPH free radical scavenging activity which increased with increasing the concentration of compounds when compared with standard drug ascorbic acid. In addition, all the compounds had effective lipid peroxidation, super oxide anion scavenging and nitric oxide scavenging depending on concentrations.

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P-60

# PROTECTIVE EFFICACY OF CURCUMIN ON IMPAIRED LIPID PROFILE INDUCED BY CADMIUM IN ALBINO MICE

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**ABSTRACT:** Cadmium (Cd), a common toxic heavy metal, is widely distributed in the environment due to its use in industry. In the industry, Cd is hazardous both by inhalation and ingestion and can cause acute and chronic toxicity. Curcumin on the other hand has a wide variety of biological activities and has protective effects against several ailments and infections. The present study was conducted to determine the cadmium induced toxicity and protective effect of curcumin in serum lipid profile of mice. Mice were divided into four groups. Group 1 mice were kept as control. Group 2 mice were given 1mg/kg bw of cadmium on alternate days. Group 3 mice were given 1mg/kg bw of cadmium on alternate days and 100mg/kg bw of curcumin daily. Group 4 mice were given 100mg/kg bw of curcumin daily and was kept as positive control. The experiment was carried out for 45 days and autopsies were done on 45 days post treatment. Blood was collected, serum was separated and lipid profile was estimated. There was significant increase in serum cholesterol, LDL-c, VLDL-c, triglycerides and significant decrease in HDL-c in cadmium treated groups in comparison to control. But in curcumin treated groups, their level were found to attain almost normal values as compared to control. Therefore, results suggest that curcumin showed preventive action since it exhibited the ability to resist the harmful action of cadmium.

**Keywords:** Cadmium, Curcumin, Protective and toxicity.

**P-61**

# Synthesis, characterization and *in-vivo* anticancer activity of some pyrimidine derivatives

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**Abstract:** A series of pyrimidine derivatives were synthesized and characterized by using FT-IR, $^{1}$HNMR [1]. The *in-vivo* anticancer study was investigated in swiss albino mice bearing Ehrlich Ascites Carcinoma (EAC) cells [2]. The synthesized compounds were administered intraperitoneally at a dose level of 35 mg/kg; body weight. 5-Fluorouracil (5-FU) was used as the standard drug. The compounds showed significant inhibition of cancer cell growth. The investigation supported the pyrimidine derivatives as the potent anticancer molecules for further study.

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P-62

# ONE-POT EFFICIENT [4+2] CYCLOADDITION ROUTE TO TETRAHYDROPYRIDINES VIA NITRENE INSERTION

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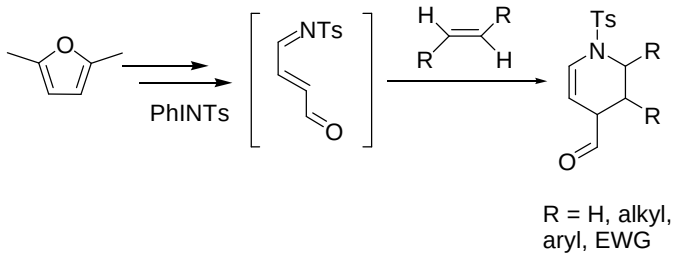
Nitrogen heterocycles are of immense importance not only as key components of a range of bioactive compounds, both naturally occurring and synthetic, but also as synthetic precursors to a variety of pharmaceutically and industrially relevant nitrogen-containing compounds.[1] In particular, tetrahydropyridines are one of the fundamental heterocycles, which have been the subject of intense research for their outstanding biological properties and wide range of applications to pharmaceutical companies and synthetic intermediates. In continuation of our ongoing efforts to develop synthetically useful heterocyclic frameworks via nitrene transfer strategy,[2] the scope and generality of the reaction was adequately investigated and the conditions were optimized extensively. The synthetic protocol presents the new one-pot [4+2] cycloaddition for the synthesis of tetrahydropyridines. Here we have synthesized some tetrahydropyridine derivatives at room temperature using 2,5-dimethylfuran, PhINTs[3] as nitrene source, $CuTp^X$ as catalyst.




**Scheme 1**

No by-product formation, atom-economy, operational simplicity, ambient temperature, and high stereoselectivity are the salient features of the present protocol, which would enhance the scope of chemical and pharmaceutical applications of tetradropyridines.

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P-63

# NOVEL INDOLE DEIVATIVES AS LIGASE-I INHIBITOR

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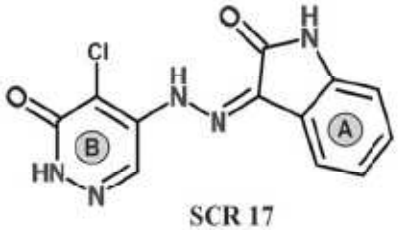
Programmed DNA replication and repair machinery ensure proper maintenance and propagation of genome under normal circumstances. A genetic defect in repair, recombination and replication process can result in increased incidence of diseases especially, cancer. Cell adopts different DNA repair pathways. NHEJ, HDR, single-strand break repair and alternative NHEJ are the commonly adopted one[1]. Although most of these pathways are essential for survival of a normal cell, they also provide advantage to cancer cells to negotiate with DNA damage. Ligase is the group of enzyme involved in single and/or double-strand of DNA repair process during replication, repair and recombination. Among them Ligase-I and Ligase-IV play vital role. Ligase-I ligates nascent DNA of the lagging strand while ligase-IV catalyses NHEJ double-strand break repair process[2,3]. Considering it's (Ligase) indispensable role in DNA repair process, a therapeutic strategy was adopted to inhibit proliferation of cancer cells by using specific small molecules as Ligase inhibitors. In present study, series of Indole derivatives were designed, synthesized and screened for their DNA Ligase-I inhibitory property. Based on biological experiments, two Ligase-I inhibitors namely, SCR17 and SCR21 were identified and found to be effective at nM range, and selective in nature.

**Key Words:** Indole, Ligase, Cancer, DNA repair.




SCR 17


SCR 21

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**P-64**

# Tandem Cu(I)-catalyzed decarboxylative/C–H activation coupling of cyclic diketones, proline and alkynes

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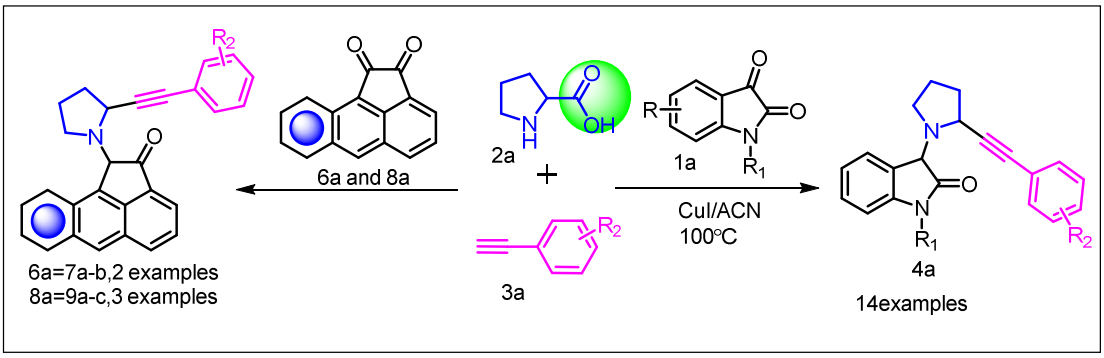
An efficient ligand/base and oxidant-free copper(I) catalyzed intermolecular direct alkynylation (IDA) strategy has been developed for the synthesis of α-alkynylated pyrrolidine-oxindole derivatives [1]. Our preliminary work has been based on organocatalysis as well as multicomponent reactions for the synthesis of various biologically important heterocyclic compounds [2,3]. In continuation of this protocol, this method adds a new dimension for the formation of α-alkynylated pyrrolidine-oxindole derivatives using cyclic diketones, amino acids and alkynes via tandem decarboxylative/C–H activation and reductive-amination strategy.

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**P-65**

## ZnO-Nanoparticle catalyzedUgi-reaction in aqueous medium

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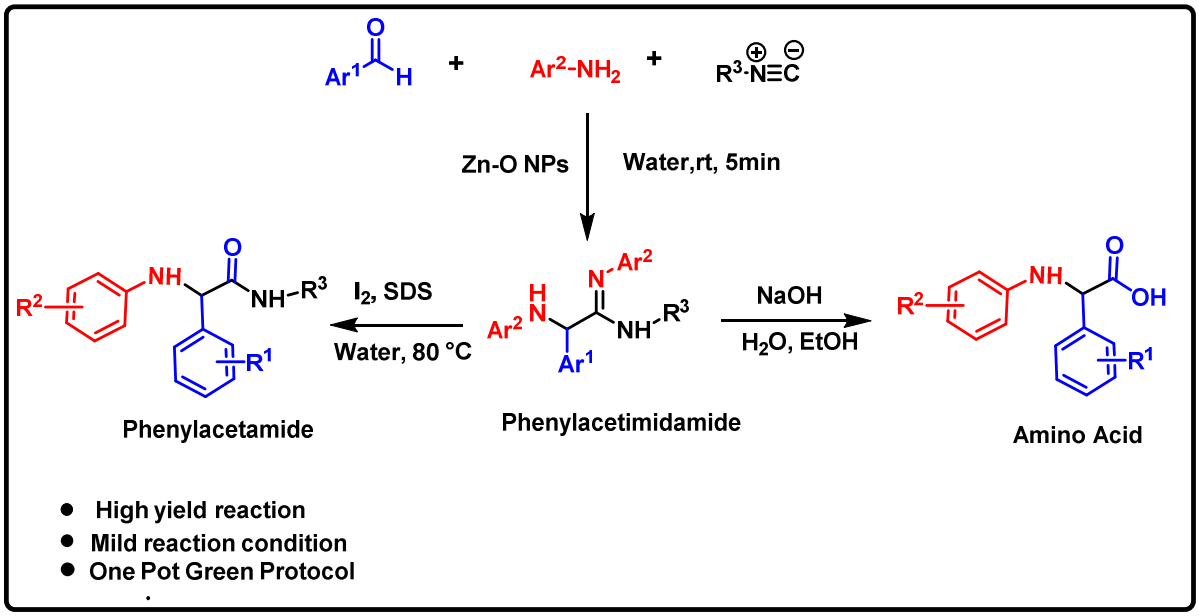
The first ZnO-NP catalysedUgi type three-component (AB2C) reaction[1]has been developed for the synthesis of 2-arylamino-2-phenylacetimidamide from an aldehyde, amine and isocyanide in aqueous media. Our preliminary work has been based on organocatalysis as well as multicomponent reaction (MCRs) for the synthesis of various biologically important heterocyclic compounds[2] [3].This nanoparticle catalysed reaction (NPCR) is high yielding and has good atom economy as well as atom efficiency. The synthesized phenylacetimidamide yielded 2-amino-2-phenylacetamide on hydrolysis with $I_2$–SDS–water, whereas alkaline hydrolysis afforded the N-substituted α-amino acid.

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P-66

# DABCO Catalysed Synthesis of 3-Substituted-3-Hydroxyindolin 2-ones in Aqueous Media

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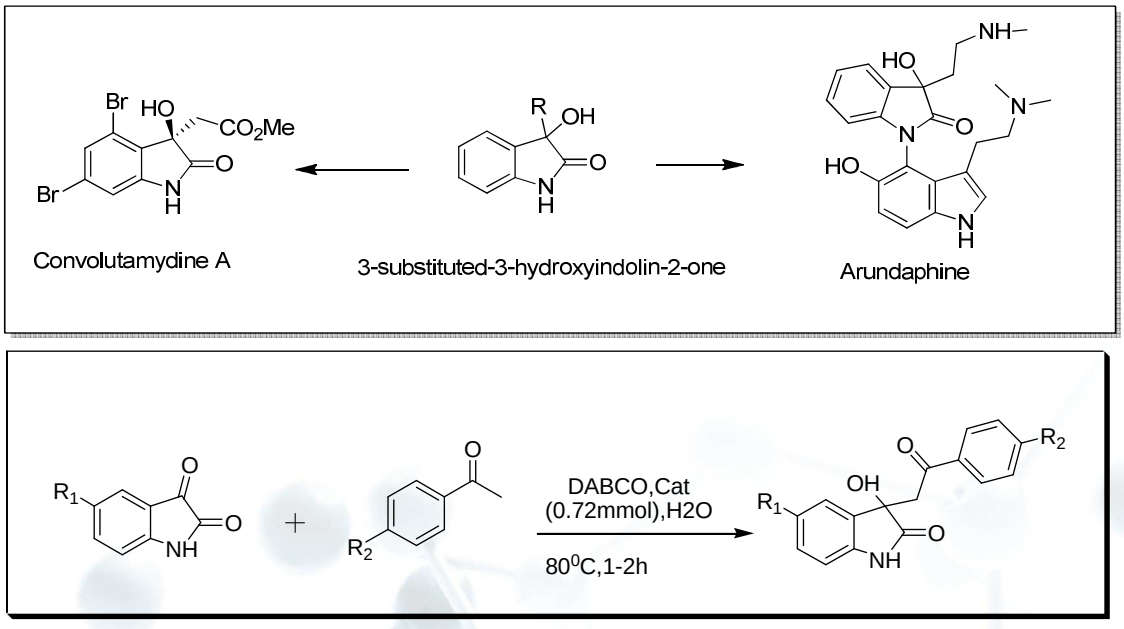
**Abstract:** The 3-substituted-3-hydroxy-2-oxindole [1]have drawn tremendous interest of researchers in the area of synthetic organic chemistry as well as drug discovery because of their occurrence in many biologically active compounds [2]We have developed a green and efficient method for an easy access of 3-substituted-3-hydroxyindolin-2-ones catalysed by DABCO. The reaction merits the shorter reaction time, high yield of theproducts and easy purification process.

There are various elegant and efficient methods for synthesizing 3-substituted-3- hydroxyindolin-2-ones in both racemic as well as chiral versions documented in the literature, but most of them have several drawbacks such as use of metal catalyst, longer reaction times, poor yields, and cumbersome workup processes. Recently, a great deal of attention has been paid to the use of water as a reaction media and it has been demonstrated as a good solvent despite having certain limitations.Water has advantages over many traditional organic solvents such as being nontoxic, easily available, and easy to handle in workup processes.

**Keywords:** Isatin, Acetophenone, DABCO (0.7mmol) and water as solvent.




Scheme- synthesis of 3-hydroxyindolin2-one

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P-67

# FORMULATION, OPTIMIZATION AND *IN-VITRO* CHARACTERIZATION OF RAMIPRIL LOADED SOLID LIPID NANO PARTICLES

REMYA .P.N, KAVITHA.R, DAMODHARAN.N

**ABSTRACT:**

Ramipril loaded solid lipid Nano particles were produced by hot homogenization followed by Ultra sonication at temperature above the melting point of lipid. SLN were characterized for entrapment efficiency ,drug content ,zeta potential, *In-vitro* drug release, particle size analysis, scanning electron microscopy, Fourier transform infrared studies and stability. The SLNs formed were in Nano size with maximum entrapment efficiency with an initial burst and prolonged release over 24h.

**OBJECTIVE:-**
Solid lipid nano particles were prepared by hot homogenization followed by ultra sonication. Stearic acid, Glycerol mono stearate were used as solid lipid core, Tween 80,Tween 40,Tween 20 were used as surfactants mixture. Process ad formulation variables were studied and optimized.

**METHODS:-**
Hot Homogenization of melted lipids ad aqueous phase followed by ultrasonication at temperature above the melting point of lipid was used to prepare SLN dispersion. The prepared formulations have been evaluated for entrapment efficiency ,drug content ,zeta potential, *In-vitro* drug release, particle size analysis, scanning electron microscopy, Fourier transform infrared studies and stability.

**RESULTS:-**
The mean particle size, PDI, Zeta Potential and entrapment efficiency of optimized Ramipril SLN formulation was found to be 37.54 nm,0.173,19.70mv,88.63% respectively. *In-vitro* release studies indicated that after an initial burst release, SLN could provide prolonged release of Ramipril

**CONCLUSION:-**
In this study a poorly water soluble drug, Ramipril was successfully incorporated into SLNs by modified high shear homogenization and followed by ultra-sonication. SLN formulations F1 ad F10 composed of Tween-80 as a surfactant ad lower concentration of lipid matrix showed the best results in view of the entrap efficiency as well as in *In-vitro* drug release.

**Keywords:** Solid Lipid Nano Particles, Ramipril, particle size analysis, entrapment efficiency, *In-vitro* release study

**P-68**

# COMPARISON OF *ESCHERICHIA COLI* STRAIN RECOVERED FROM URINARY TRACT INFECTED HUMAN URINE SAMPLE WITH LABORATORY *E.COLI* STRAIN

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**ABSTRACT:** Urinary tract infection is one of the most common types of nosocomial bacterial infection and because of its high incidence, it is responsible for an enormous aggregate burden of morbidity, mortality and increased healthcare costs. Here we sought to compare the pathogenic characters of the organism from the urinary tract infection with the normal laboratory organism. In the present study urine sample collected from urinary tract infection symptom patients in SRM Hospital and Research centre, Chennai, Tamil Nadu. By using Macconkey agar and EMB agar medium,Organism was isolated from urine sample, from the biochemical characterization; we found that the isolated organism may be *Escherichiacoli*. Pathogenic character of isolated uropathogenic organism was found by their haemolysin production. It showed halo in sheep blood agar medium, because of presence haemolysin. The protein from both strains was purified by dialysis method. After isolation SDS-PAGE electrophoresis was performed for both protein and compared the presence of Proteins in both organisms. Its shows change in their protein bands.Genomic DNA of the uropathogenic E.coli and NICM E.coli strain showed same pattern of DNA band after staining with ethidium bromide.From the results we concluded that the pathogenic character of uropathogenic E.coli strain is due to the haemolysin production. Further study has to be carried out the DNA finger printing of the uropathogenic strain and can compare the sequence with the NCIM strain for to find the genomic difference between two strains.

**Key Words:** *Escherichia coli*, UTI bacteria, SDS-PAGE

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**P-69**

# Synthesis characterization of Indolizine derivatives for antioxidant activity

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The indolizine ring is an important structural moiety with interesting and promising biological properties,different approaches has been developed for the synthesis.In this work we are reporting the synthesis of Indolizine 3- carbaldehyde by using picoline Ethylbromopyruvate in alcohol reaction proceed smoothly and ring closure with aqeous sodium hydrogen carbonate to yield indolizine 2-carboxylic acid which is heated with calcium oxide to give indolizine and this indolizine is formylated by using DMF,phosphorus oxychloride to give indolizine 3- cabaldehyde.substituted 1,3,4 thiadiazole 2- amine synthesized by substituted carboxylic acid with thiosemicarbazide and fused with indolizine carbaldehyde which characterized by IR, $H^1$ NMR and Mass spectral data. Synthesized derivatives are screened for antioxidant activity.

**Key words:** Indolizine, antioxidant activity, thidiazole

P-70

# HEPARIN BINDING AND CATIONIC SMALL INHIBITORY EFFECTS ON HEPARIN INTERACTING PEPTIDE

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**Abstract:** Heparin interacts with a number of proteins, thereby playing vital role in the regulation of numerous physiological processes [1]. Various biophysical methods such as ITC, SPR, CD, AFM were employed to study the interaction between HIV-1 TAT peptide (Heparin Interacting Peptide) and heparin. TAT is a regulatory protein released by HIV-infected cells which is responsible for viral replication [2]. The investigation was focused on understanding the type of interactions driving the mechanism of HIP-heparin complex formation, and also exploiting the possibility of using cationic small molecule as inhibitor of HIP-heparin complex. Analysis based on isothermal titration calorimetry (ITC) of HIP-heparin interactions suggests that binding takes place in two stages. The contribution of ionic interaction (22%) was found to be very small to the overall binding affinity, and interaction stands out clearly from a random, nonspecific binding. Atomic force microscopy images (AFM) confirmed complex formation between heparin and HIP. ClusPro docking software successfully predicted HIP as major heparin binding site in Tat proteins. Quinacrine, which was used to test modulation of HIP-heparin interactions, exhibited successful inhibition of these interactions in ITC and SPR. Circular dichroism studies confirmed that quinacrine upon binding induces alteration in heparin conformation leading to peptide inhibition. These results demonstrate the feasibility of modulation of heparin-protein interactions which could be effective strategy for the development of therapeutic agents.

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**P-71**

# Exploration of novel natural compound inhibitors against *Plasmodium falciparum* Dihydroorotate dehydrogenase (*Pf*DHODH): A computational approach

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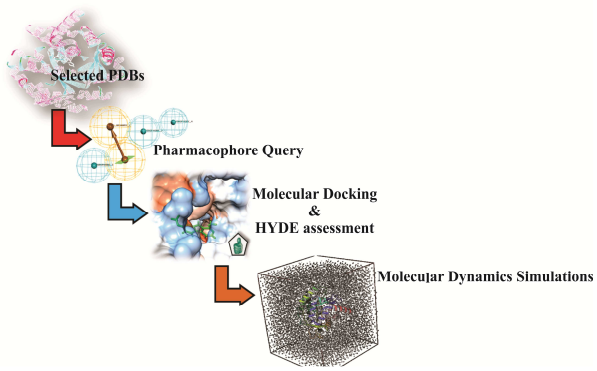
**Abstract:**




Malaria is considered as one of the major public health concernwhich resides in human civilization since long ago. [1] Among the five *Plasmodium* species, *Plasmodium falciparum* (*Pf*) is accountable for most of the malarial cases. [2] However, the emergence of resistance to all major chemotherapeutic drugs has emphasized the need for effective prophylactic means. [3, 4] As a result of past research, it is quite clear that an improved chemotherapeutics offering efficient and consistent protection is of high national and international importance.

Taking account of the challenges, Dihydroorotate dehydrogenase (DHODH) seems to be a logical and attractive choice as its activity plays a crucial role in bacterial viability. [5, 6] In this pursuit, a novel methodology was adopted for the construction of common hypothesis pharmacophores (CHP's) utilizing the *Pf* structural proteome. The retrieved hypotheses were rigorously validated and the top scored modelwas then employed to prioritize the molecules from SPECS natural product database.Moreover, the auxiliary evaluation of the retrieved candidate molecules was carried out by couplingthe docking studies with HYDE assessment.Furthermore, the molecular details of binding interactions of the potential hits were envisioned via molecular dynamics simulations in order to list the possible candidate that can be targeted against *Pf*DHODH. The efforts led to the identification of a novel inhibitors presumed to be more potent against *Pf*DHODH. We look forward to experimentally validate our computational results.

**Keywords:** Malaria; *Plasmodium falciparum*; docking; molecular dynamics simulations.

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P-72

# MICROWAVE ASSISTED SYNTHESIS OF QUINOLINE-4-CARBOXYLIC ACIDS AND THEIR *N*-GLYCOCONJUGATES

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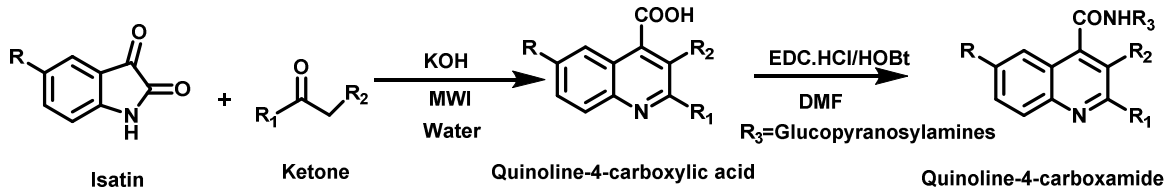
Pfitzinger condensation reaction of isatins with α-methylene carbonyl compounds is an efficient procedure for synthesising active derivatives of quinoline-4-carboxylic (cinchoninic) acids (QCA). The quinolone pharmacophore has many medicinal applications, such as antimicrobial, HIV-1 integrase inhibitors, antitumor and antiviral activities [1]. In our synthetic strategy we employed substituted isatins with various ketones in the presence of a base using water as a solvent to get substituted quinoline-4-carboxylic acids in moderate to good yields under Microwave Irradiation (MWI) for 10-12min.Furthermore, we applied the same synthetic procedure for synthesising quinoline-4-carboxylic acids containing various heterocyclic moieties like pyridine, thiophene, etc. After synthesising a library of quinoline-4-carboxylic acid derivatives we extended our work for synthesising biologically important carboxamide derivatives of those acids using coupling reagents like EDC.HCl, and HOBt. We used various amine groups starting from simple anilines to various substituted amines. Importantly, we were able to couple our QCAs with glucopyranosylamines [2] to synthesise amino acid derived *N*-glycoconjugates. The latter have been reported as excellent anti-inflammatory agents.

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P-73

# Development of Nitromethane catalyzed C-H activation for the preparation of chromeno[3,4-*d*]imidazol-4-ones as hybrid scaffolds

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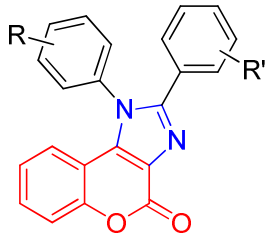
**Abstract:** Designing of novel drug molecules involve multiple parallel and intersecting approaches; however bio-inspired design process and rational design process have been two major directions to work at, during last few decades. At the border between bio-inspired design and rational design, one can imagine preparation of hybrid molecules with a dual mode of action to create efficient new drugs. In this account, hybrid molecules can be defined as chemical entities with two or more structural domains having different biological functions and dual activity, indicating that a hybrid molecule acts as two distinct pharmacophores (a "double edged sword").

Herein we report a tandem cyclization protocol towards hitherto unprepared hybrid scaffolds of coumarin and imidazole core. The synthetic methodology initiates with linking of aromatic amines with coumarin at 4-position, followed by tandem cyclization with the help of nitromethane leading to the synthesis of title compounds in high to excellent yields (80-97%). Detailed characterization including $^{1}$H NMR, $^{13}$C NMR and HRMS for all newly synthesized compounds has been reported.




**20 examples**
**85-90% isolated yield**

**P-74**

## Structure-Activity Relationship of Dual Active New Generations Fluoroquinolones

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The frequent, inappropriate use of the broad spectrum, potent class of fluoroquinolone antibiotics leads to the rapid development of resistant bacterial strains against current fluoroquinolones posing a serious concern in medicine and in the global health scenario. Therefore, we have developed new counter-strategies of "Dual Action Rational Therapeutics" (DART) that involve rational structure-based drug design approach to generate a library of new fluoroquinolones with multi-mode activities to bypass and/or suppress fluoroquinolone resistance. In one of the strategies we havesynthesizednovel fluoroquinolone conjugates,incorporated different nitro-heterocyclic motifs to the C7 piperazine moiety with suitable tethers. Our aim is to determine the particular nature of a nitro-heterocyclic motif that wouldresult higher DNA-gyrase binding and potent activity against both susceptible and resistant *Staphylococcus aureus*. All these molecules have found to retard emergence of resistance in different extent proved by *in vitro* emergence of resistance studies. Nitrofuran based fluoroquinolones showed promising tendency to retard emergence of resistance as well as showed broad spectrum of activity in comparison to nitro-thiazole and nitro-imidazole based fluoroquinolones against *S. aureus*. Thus in silico and *in vitro* analysis of these fluoroquinolones revealed that the nature and mutual spatial orientation of different nitro-hetrocyclic motifs with respect to the fluoroquinolone nucleus is a crucial determining factor for maintaining multi-functionality of the final molecule with enhanced DNA-gyrase binding interaction. Designing this library of molecules has provided an opportunity to select an effective fluoroquinolone skeleton to finally obtain "drug candidates" with improved PK/PD profile and limited toxicity for the treatment of specific local/topical infections caused by fluoroquinolone resistant Gram positive and Gram negative pathogens.

**P-75**

# Hepatoprotective activity of Ethanol extract of *Amaranthus viridis* Linn and its evaluation of Hepatocellular carcinoma on Aflatoxin B1 induced rats.

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**Abstract:** The ethanol extracts of *Amaranthus viridis Linn (EEAV)* and its evaluation of hepatocellular carcinoma induced by Aflatoxin B1 (AFB1). AFB1causes oxidative stress and enhanced formation of reactive oxygen species (ROS) and is associated with increases in biochemical parameters like Serum glutamyl pyruvate transaminase (SGPT), Serum glutamyl oxaloacetic acid(SGOT), Serum alkaline phosphatase (SALP), Glutamyl transpeptidase (GGT), Bilirubin, Lipid levels as well as decrease in the levels of total protein and uric acid. EEAV was administered orally (100 & 200 mg/kg) for 14 days to hepatocarcinoma bearing rats. The levels of lipid peroxides and activity of enzyme antioxidants level were determined in liver homogenates. Marked increase in lipid peroxide levels and decrease in enzymatic antioxidants levels were observed in carcinoma induced rats, while EEAV treatment reversed the conditions to near normal levels. Liver histopathology showed that EEAV reduced the incidence of liver lesions, lymphocytic infiltrations and hepatic necrosis induced by AFB1 in rats. These results suggest that EEAV could protect liver against the AFB1-induced oxidative damage in rats, which may be due to its capability to induce them *in vivo* antioxidant system.

**Key words**: Hepatocellular carcinoma, Aflatoxin B1, *Amaranthus viridis Linn*, Reactive oxygen species.

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# Design and microwave assisted synthesis of novel 2-phenyl/2-phenylethynyl-3-aroyl thiophenes as potent antiproliferative agents

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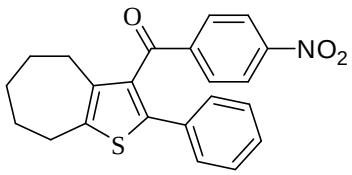
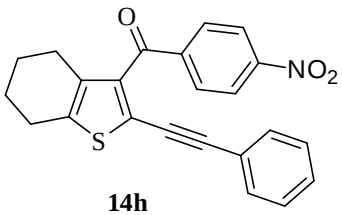
Despite the significant progress achieved in chemotherapy, cancer is still among the leading causes of morbidity and mortality worldwide, with approximately 14.1 million new cases of cancer diagnosed every year and this number is expected to further increase to over 22 million within the next two decades [1]. The narrow therapeutic indices of anticancer drugs and the problems of chemoresistance and toxicity to normal cells are the major hurdles in the effectiveness of anticancer therapy. This necessitates the search for the development of novel, safe and more effective chemotherapeutic agents [2]. Polysubstituted thiophenes have attracted excessive attention due to their pronounced anticancer properties [3-4]. In the present study, 2-phenyl/2-phenylethynyl-3-aroyl thiophenes have been designed and synthesized *via* microwave assisted methods. All the synthesized compounds were evaluated for *in vitro* antiproliferative activity against various human cancer cell lines. Compounds **12j** and **14h** were found to be the most promising compounds against all the tested cancer cell lines, particularly against A-375 ($IC_{50}$ = 1.07 ± 0.1 and 0.81 ± 0.1 µM, respectively) and MIA PaCa-2 ($IC_{50}$ = 5.35 ± 0.6 and 3.00 ± 1.0 µM, respectively) cancer cell lines, which are comparable to the standard paclitaxel. Further, the antiproliferative activity of the most potent compounds **12j** and **14h** was confirmed by calcein AM and clonogenic assays and was found to induce cell cycle arrest at the G2/M phase, suggesting that cell exposure to selected derivatives produces mitotic failure. *In silico* ADME studies confer the oral drug like characteristics of the potent compounds.




**12j**




**14h**

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# Design, synthesis and biological evaluation of novel dual inhibitors for the treatment of Alzheimer's disease

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Alzheimer's disease (AD) is a multifactorial progressive neurological disorder characterized by loss of memory due to decrease in the cholinergic transmission in the brain. About 5.4 million Americans of different age groups are estimated to be living with AD as of 2016[1]. There is practically no drug for the treatment of AD that can address the basic pathophysiological factors responsible for the disease.

Matrix metalloprotease (MMPs) are involved in the normal cell signalling processes of inflammation, amyloid beta aggregation and angiogenesis. Several studies suggest that MMP enzyme is a promising new target for the treatment of AD. Among the MMPs, the level of MMP-2 and 9 is increased in AD patiens[2]. Recently, it has been shown that AChE is one of the key proteins co-localized with Aβ deposits and modulates the formation of toxic species.

Our hypothesis is to develop *in-vivo* active novel dual inhibitors of MMP2/9 and selective AChE inhibitors with an ability to address basic factors responsible for the disease. To achieve this, we are planning to design hybrid drugs incorporating necessary pharmacophoric features required for interaction with enzyme and to provide multifunctional property in a single molecule.

In the present study, hybrid drug development approach is being explored for the desing of novel sulfonamide analogs[3]. We are exlproing the role of hyrdophibicity for enzyme inhbition and amyloid beta aggregation modulation. Therefore, various substitued biphenyl fragments are appdended to heterocylcic rings using a suitable linker. The compunds are being syntheszied using the art of synthetic medicinal chemsitry and fully charactreized with help NMR. The detail biological evaluation including the enyzme inhibions assays, cytotoxocity and molecualr docking results will be presented. Author are thankful to DBT and IIT(BHU).

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**P-78**

# Enantiomer self-disproportionation (ESD) for the separation of non-racemic mixtures

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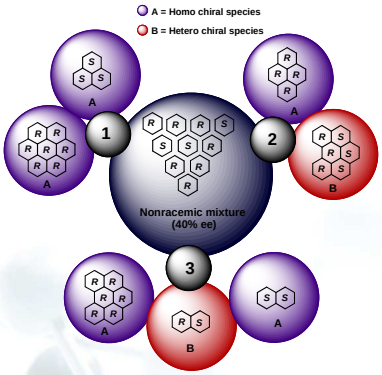
Chirality plays key role in the modern pharmaceutical industry, asymmetric synthesis, reaction pathways and agrochemical industry. As body being enantioselective, it will react with each racemic molecule by a diverse stereo-specific mode to generate dissimilar pharmacological activity. Wherein, one enantiomer may make the desired therapeutic effects, while the other isomer remains inactive or give unwanted effects. This interest can be attributed largely to the principle awareness that isomers of a racemic pharmaceuticals may have dissimilar pharmacological activities. Currently, a majority of commercially available medicines are both synthetic and chiral in nature. However, a plenty of chiral medicines are still traded as racemic mixtures. Therefore, there is a great demand to build up new technologies for analysis and separation of racemic pharmaceuticals. Chiral chromatography is one of the advanced methods for enantiomer separation. Recently, an interesting phenomenon of enantiomers self-disproportionation (**ESD**) has been reported by Soloshonok et al. [1-2] using achiral silica gel (Figure). Additionally, Mayani et al. [3-4] has invented the third possible mechanism of ESD phenomenon. Our present work primarily deals with **ESD** of commercially important chiral compounds as analytes using different eluents with achiral stationary phases namely nano silica ball (**NSB**) and nano carbon cage (**NCC**). The enantiomers of mandelic acid, 1-(4-fluorophenoxy)-2-propanol, 4-fluoro-alpha-methylbenzyl alcohol, 4-flurophenyl oxirane, BINOL, cyanochromene oxide and 2-phenyl propionic acid were successfully separated to some extent using enantiomer self-disproportionation phenomenon. ESD is highly dependent on the nature of the compounds and its optical purity. It is therefore can be concluded that it is not safe to assume that any type of chromatography is a reliable method for the purification of a non-racemic mixture of a chiral compound, as chiral purity of the pre-purified sample may differ drastically after chromatographic purification.

***Keywords*:** Chirality, Enantiomer Self-disproportionation, Non-racemic, Achiral Silica Carbon

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P-79

# Development of sustainable Au (III) Salen complex doped carbon nanocomposite for catalytic degradation of hazardous pollutant dyes

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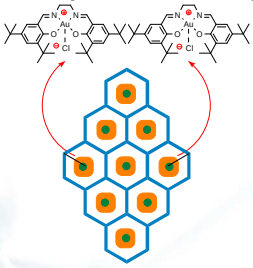
Huge amounts of wastewater containing compounds hazardous to the environment are produced each year. Among these products, dyes are of a great importance due to its presence in textile, dyeing, printing and fertilizing industries, among others. Dyes in wastewater undergo chemical changes, consume dissolved oxygen and destroy aquatic life. The color and high COD of these effluents may cause serious environmental problems. An effective degradation and detoxification method is therefore needed to remove the toxic or carcinogenic dye residues and their by-products, which is an important issue in the field of wastewater treatment [1]. Many investigators have made great effort to study different techniques for removal of dyes and carcinogenic pollutants in wastewater. Now, various types of technologies are available such as chemical coagulation, cold point extraction, micellar enhanced ultrafiltration, nano filtration and adsorption on to kaolinite, activated agricultural solid waste, various types of activated carbon and magnetic nanoparticles. Eosin-Y, a heterocyclic dye containing bromine atoms, is used in the fields of dyeing, printing, leather, printing ink and fluorescent pigment. The direct release of wastewater containing Eosin-Y will cause serious environmental problem due to its dark color and toxicity [2]. Chromotrope-2R (C2R) is a monoazo dye with several applications in textile industry. Azo dyes represent about one-half of dyes actually used in the textile industry and, as a consequence, a relevant problem is related to the release of these products in the environment [1]. In continuous of our development of eco-friendly catalysts [3-4], the present study provides a complete perspective of gold-Salen doped carbon, **Au(Salen)CC,** for catalytic degradation of hazardous pollutant dyes viz., Eosin-Y & Chromotrope 2R, using mild reaction condition. New **Au(Salen)CC** was developed by easy methodology using nano carbon cage (CC) prepared from economical Pyrolysis fuel oil (PFO) Pitch residue. This ecological catalyst delivered significant degradation activity compared to existing reports. The heterogeneous catalyst recycled and reused successfully for four repeated experiments without loss in its adequate performance. **Au(Salen)CC** can be further utilized for new multifunctional applications as well.

**Keywords:** Eco-friendly Heterogeneous Catalyst, Hazardous pollutants, Gold-Salen Nanocomposite



Au (III) Salen on CC

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**P-80**

# Benzotriazole Ring Cleavage (BtRC) Approach for the Synthesis of diverse Benzo-fused Aza-Heterocycles

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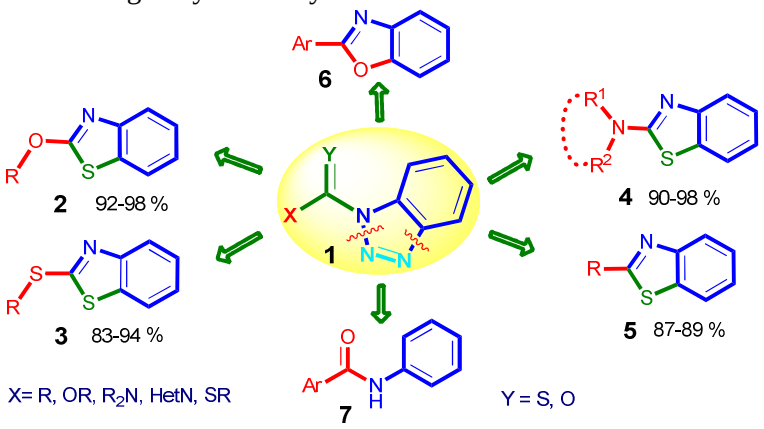
The advantages associated with utilizing benzotriazole as a synthetic auxiliary lies in enabling rather common transformations to be formed efficiently, quickly, and inexpensively. Its benign bio-physical properties, and ready availability, have placed benzotriazole methodology among some of versatile, useful and among the most successful synthetic protocols investigated so far. In present abstract, we have briefly outlined the opportunities and scope of benzotriazole ring cleavage strategy for the synthesis of benzo-fused aza-heterocycles ongoing in our laboratory.[1-4]

The benzotriazolemethanethione conjugates (**1**), on treatment with silanes or stannane under heating or microwave irradiation undergoes free radical *β*-scission of *N-N* bond and affords diverse range of 2-substituted aza-heterocycles (**2-6**) *via* cyclative-elimination of molecular nitrogen (Scheme 1).[5,6] The analysis and characterization of the synthesized compounds is based on spectral *viz*, IR, MS, HRMS, $^{1}H$, $^{13}C$ NMR and single crystal X-ray studies.




**Scheme 1.** Synthetic scope of benzotriazole ring cleavage strategy

The synthesis of 2-*O*-aryl/alkylbenzothiazoles (**2**), 2-(aryl/alkylthio)benzothiazoles (**3**), 2-(*N*,*N*-dialkyl)benzothiazoles (**4**), 2-aryl/alkylbenzothiazoles (**5**), 2-arylbenzoxazoles (**6**) and N-phenylamides (**7**) *via* benzotriazole ring cleavage using $(TMS)_3SiH$ as radical reducing agent is not realized so far, thus, this approach should be of further interest to synthetic and medicinal chemists. The short reaction period, simple workup, high yield, and mild condition of this methodology express significant tolerance towards a number of functional groups such benzylethers, acetals, thioethers, esters, arylhalogens (Ar-F and Ar-Cl), and alkenes.

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**P-81**

# Microwave assisted one-pot synthesis of novel □-D-allosyl linked heterocyclic compounds through 1,2,3-triazoles

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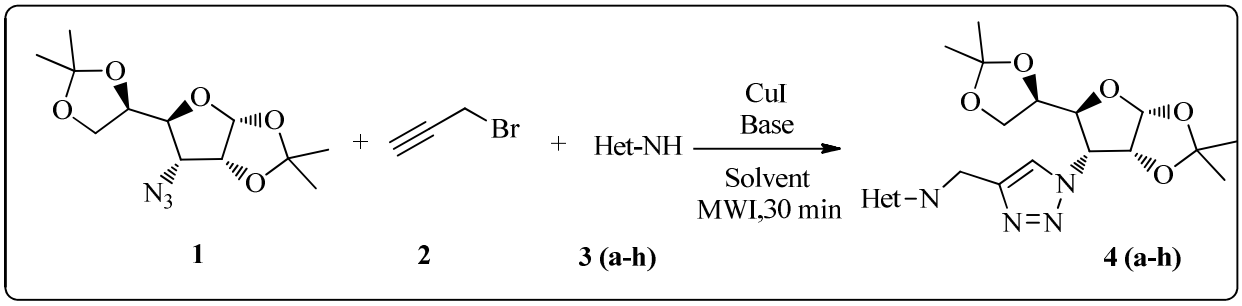
**Abstract:** A series of α-D-allosyl linked heterocyclic compounds containing 1,2,3-triazoles were synthesized by copper catalyzed one-pot three component 1,3-dipolar cycloaddition of α-D-allosyl azide, propargyl bromide with different N-heterocyclic compounds under microwave irradiation. All the synthesized compounds were characterized by NMR, IR, Mass, and elemental analysis.




***Keywords:*** One-pot MWI; α-D-allosyl; N-Heterocycles; 1,2,3-triazole.

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**P-82**

# Tetra-*n*-butyl ammonium fluoride (TBAF) catalyzed convenient synthesis of 2-arylbenzothiazole in aqueous media

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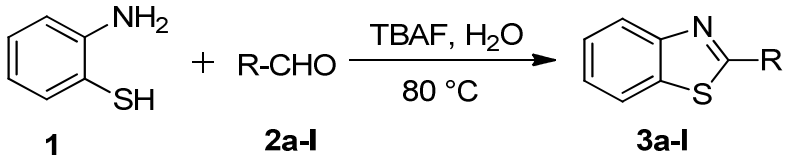
**Abstract:** A new and efficient protocol was developed for synthesis of benzothiazoles using Tetra-*n*-butyl ammonium fluoride (TBAF) as a catalyst under environmentally friendly conditions. The developed synthetic protocol represents a novel and very simple route for preparation of 2-substituted benzothiazole derivatives (3a-i) . In addition, a microwave irradiation technique is successfully implemented for carrying out the reactions in shorter time.




**Scheme -1**. TBAF catalyzed synthesis of 2-arylbenzthiazoles

**Keywords**: Benzothiazoles, TBAF, Microwave irradiation, Green protocol

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P-83

# Metal-free Regioselective C-N and C-O Bonds Formation with the Utilization of Diaryliodonium Salts in Water

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C–N and C–O bond-forming reactions have recently gained paramount importance among the scientific community for different drug-discovery and development programs. Particularly, *N*-arylated quinolones, acridones and *O*-arylated quinolines have proved to be important building blocks for the creation of broad range of compounds, including natural products, pharmaceuticals and advanced materials [1]. *N*- and *O*-arylated compounds are most commonly synthesized from transition-metal-catalyzed cross-coupling reactions such as copper-catalyzed Ullmann-type coupling or palladium-catalyzed Buchwald–Hartwig coupling [2]. Subsequently many other groups reported the metal-catalyzed as well as metal free carbon–heteroatom bonds formation reactions [3]. The use of metal-free and greener reaction conditions to avoid transition-metal-catalyst is an attractive research goal for many groups. In recent years, diaryliodonium salts have been employed as arylating agents in many coupling reactions because of their attractive and benign features such as stable solids, high electrophilicity, less toxic, and recyclability [4]. Due to potent pharmacological properties linked with arylated heterocycles, very recently we have demonstrated synthesis of 2-arylindoles, diarylsulfones, arylated azaheterocycles and *O*-arylated quinolines using diaryliodonium salts [5]. Owing to significant properties of quinolones and utilities of diaryliodonium salts, we have developed a metal-free arylation of quinolones in water by utilizing diaryliodonium salts. Prepared compounds were well characterized by NMR ($^{1}$H & $^{13}$C), IR and mass spectral data. Details about the reaction optimization, synthetic strategy and mechanistic pathway will be present in the conference.

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**P-84**

# Synthesis and Identification of *β*-Carbolinium Salts as Novel Cytotoxic Agents

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*β*-Carboline and related compounds have been abundantly found in plants, marine organisms, insects, mammalian including human tissues and body fluids in the form of alkaloids and hormones [1]. Several natural and synthetic *β*-carbolines are ascribed with broad spectrum of pharmacological properties such as sedative, anxiolytic, hypnotic, antioxidant, anticonvulsant, antiviral, antiparasitic, antimicrobial and antitumor [2]. Especially, *β*-carboline derivatives have been reported to exhibit promising antiproliferative activities against several human cancers through apoptosis induction, DNA intercalation, and CDK, topoisomerase-II inhibition [3]. In addition, a certain level of water solubility is essential for nitrogen heterocycles to be applicable for biological studies [4]. Recently, many water soluble cationic azaheterocycles have been identified as potent antitumor agents [5]. Our continuous research efforts to identify potent indole-based anticancer entities [6] and inspired by the interesting anticancer potential of *β*-carbolines and azolium salts, we have designed and synthesized a series of twenty *β*-carbolinium salts for their cytotoxicity studies. *β*-Carbolinium salts were achieved by the reaction of *β*-carbolines with 1-aryl-2-bromoethanones in ethanol under microwave irradiation. Structures of the synthesized compounds were confirmed by NMR ($^{1}$H & $^{13}$C), IR and mass spectral data. Prepared *β*-carbolinium salts were evaluated for their cytotoxicity against a panel of six cancer cell lines. *In vitro* cytotoxicity study led to identify some potent *β*-carbolinium salts with $IC_{50}$ values in low micromolar range against tested cancer cell lines. One of the most potent analogue was found to be broadly active against all the tested cancer cell lines ($IC_{50}$ = 3.16-7.93 µM). Preliminary mechanistic studies disclosed that cell death on castration resistant prostate cancer cell line (C4-2) resulted in increased levels of cleaved PARP1 and AO/EB staining, indicating that *β*-carbolinium bromides induce apoptosis in these cells. Design, synthesis, structural elucidation and cytotoxicity of *β*-carbolinium salts will be discussed during the presentation.

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P-85

# Copper and Palladium Catalyzed Consecutive-Operation: Direct Synthesis of Functionalized Azepino Fused Isoindol-14-ones

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Copper and palladium catalyzed cross coupling reaction are uniquely suited to lead the new C-C and C-N bond formation.[1] These new bonds are requisite to facilitate the constructionof *N*-fused heterocycles.[2]There are number of biologically active natural products and pharmaceuticaldrugs which contain *N*-fused fused complex heterocycles.[3]Owing to their outstanding contribution, developing novel fused heterocycles by straightforward synthetic routesare always in demand. Thus, our research mainly concerned withaza-fused heterocycles through transition metal catalyzed cross-coupling reactions.[4] In the series of developed aza-fused heterocycles, we developed an efficient method for the synthesis of azepinoisoindolone derivatives*via* copper and palladium catalyzed consecutive operation. Details of the protocol will be presented in the poster.

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**P-86**

# Copper-Catalyzed Deformylative Coupling of Cinnamaldehydes Derivatives and Naphthols

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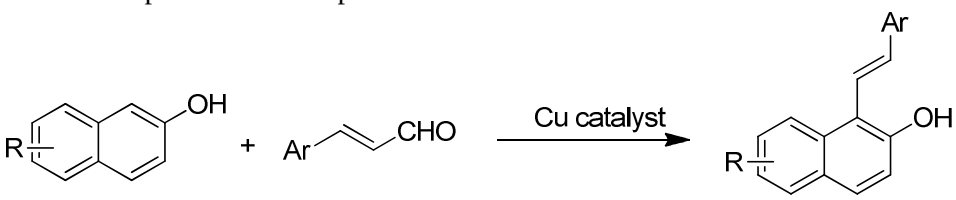
Transition metal-catalyzed coupling reactions have demonstrated great potential in synthetic organic chemistry, and has evolved as an indispensable synthetic tool.[1]However, there still lies scope for the development of newer approaches employing different reaction partners in place of pre-functionalized aryl halides/organometallic reagents. In this regard, transitionmetal-catalyzed decarboxylative couplings reactions have received great attention of organic chemists owing to their potential advantages, such as easy availability, selectivity, and high efficiency.[2] Recently, aldehydes have been employed as precursors for(oxidative) decarbonylative coupling reactions catalyzed by ruthenium or rhodium.[3]With our interest in transition metal catalyzed C-H functionalization,[4] we investigated reaction of cinnaladehydes with naphthols using different metal catalysts and found that copper based catalysts resulted in excellent yield of deformlative coupled product (**Scheme 1**). Details of the protocol will be presented in the poster.




**Scheme 1**

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P-87

# Organocatalytic one-pot approach towards the synthesis of tri substituted pyrrole ring systemsthrough [3+2] annulation/ $I_2$ mediated oxidation

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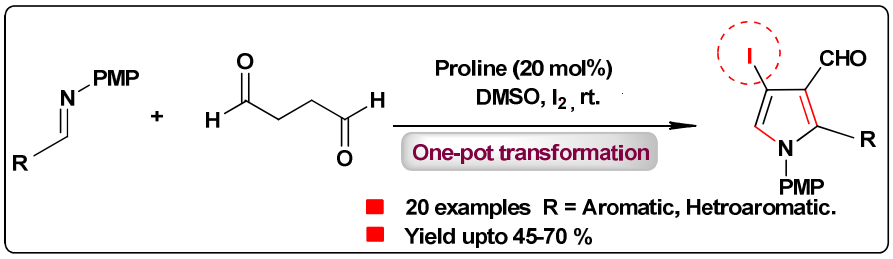
**Abstract:** The pyrrole nucleus is widespread in nature and the key structural fragment of heme(hemoglobin) and chlorophyll[1].Pyrrole moietypresent in numerous biologically active natural products such as antiviral, anti-tumor, anti-oxidative, anti-inflammatory drugs[2]. Synthesis of pyrrole ring system has been attracted great attention of synthetic chemist in recent years[3].In continuation of our interest in organocatalyzed reactions, using linear dicarbonyl compounds as *donor-acceptor* precursors, recently, we developed an efficient organocatalytic method using succinaldehyde as 1, 3-carbon dipole and imines for the synthesis of 2,3- disubstituted pyrroles in high yields (up to 82%)[4]. The present idea of succinaldehyde as 1, 3- carbon dipole with imines through [3+2] annulation followed by via $I_2$mediated one pot oxidation protocol is very compatible and even more greener as compared to the methods known earlier[5]for the synthesis of 2, 3, 4-trisubstituted pyrroles from 1,4- dicarbonyl compounds(2, 3-disubstituted 4-iodo pyrroles).4-iodo pyrroles have been found asa useful synthetic substrates for the synthesis of biologically important heterocycles[6].Organocatalytic[3+2] annulation of succinaldehyde with imines followed by $I_2$ mediate oxidation for the regioselective synthesis of 2, 3-disubstituted 4-iodo pyrroles in one pot will be presented here.This method can be further utilized for the synthesis of some small molecule natural products. (**Scheme 1**).




**Scheme 1**: Organocatalytic [3+2] annulation followed by iodine mediated oxidation sequence for the synthesis of 2, 3-disubstituted 4-iodo pyrroles

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**P-88**

# Synthesis, characterization, crystal structure of RNA targeted L- and D-phenylalanine-(1, 10-phen)-copper(II) conjugate complexes; Comparative *in vitro* RNA binding profile of enantiomers and their biological evaluation by morphological studies and antibacterial activity

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New ternary chiral Cu(II) complexes **1a** and **b** derived from L- and D-phenylalanine and 1, 10-phenanthroline were synthesized and characterized thoroughly by single crystal X−ray diffraction and other spectroscopic techniques *viz*., UV−vis, IR, EPR, ESI−MS and elemental analysis. Complexes crystallized in the monoclinic *P21* space group. Comparative *in vitro* RNA binding studies of L– and D–enantiomeric complexes were carried out by a variety of optical spectroscopies *viz.*, UV−vis, fluorescence, circular dichroism and since copper being a redox metal ion, cyclic voltammetry was employed to evaluate the enantioselective RNA binding. [1] The results demonstrated that L–enantiomer of Cu(II) complex binds more avidly to t–RNA motif in comparison to D–enantiomer with respect to comparative $K_b$, $K$ and $K_{sv}$ values of L– and D–complexes. SEM analysis divulged surface morphological alteration of complexes, evidenced by the formation of hollow tubes and concrete like structure with RNA condensate which was less pronounced in SEM micrographs of D–enantiomer condensate. Antimicrobial activity of complexes **1a** and **b** carried by agar well diffusion method demonstrated significant antibacterial activity. [2]

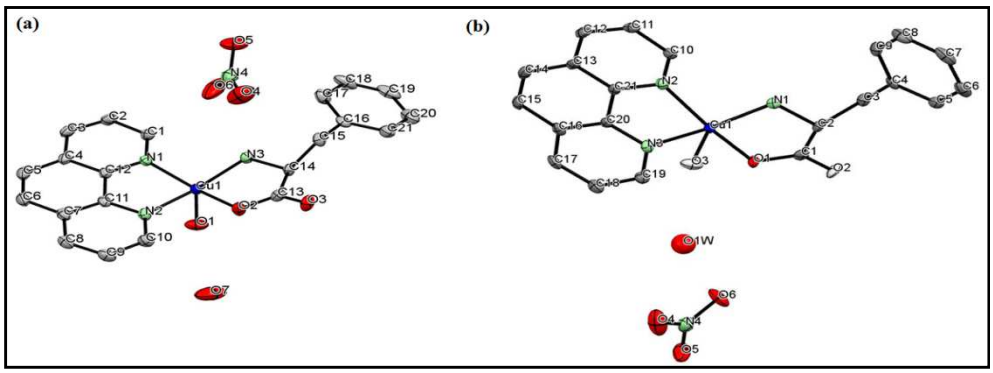


**Fig. 1** *ORTEP view of* ***(a)*** *complex* ***1a,*** *L-enantiomer and* ***(b)*** *complex* ***1b,*** *D-enantiomer with partial numbering. Solid thermal ellipsoids are reported at the 50% probability level. Hydrogen atoms have been omitted for clarity.*

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**P-89**

# Structural Transformations of Coordination Polymers on the Counter Anion Exchange and Metal-metathesis

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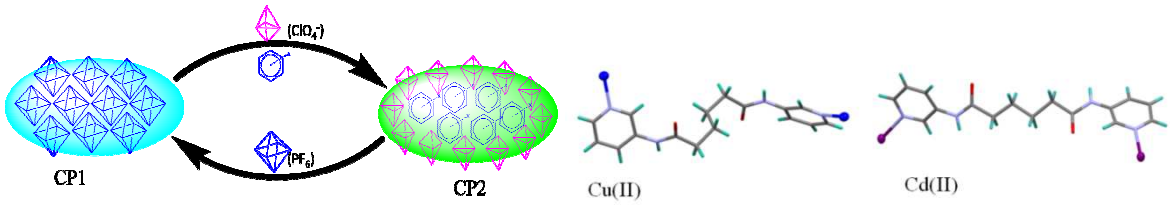
**Abstract:** Crystal engineering of Coordination-polymer (CP)s is attracting much attention since past two decades for their potential applications in the areas of gas storage, molecular sensing, separation, catalysis, etc. The cogent design of CPs can be in principle controlled through the judicious selection of metal nodes and the organic linkers. In contribution to this we analyzed the ways to design stable and flexible CPs that can show structural transformations in response to the external stimulus such as counter anions, guest molecules. For this reason in our current work we synthesized the CPs with bispyridyl-bisamide ligands with alkyl group in the spacer. Amide functional group is a promising functional group for its ability to provide stable and flexible network geometries with softer but network directing hydrogen bonding interactions and the alkyl group in the spacer generates the dynamic nature to the CPs due to its conformational changes. The main focus in this work is to determine the different CPs with the response of ligand to the respective metal nodes, effect of different types of counter anions in directing the flexible alkyl chain of CPs to adopt different conformations there by affecting the guest inclusion properties and the metal-metathesis to get CPs with desired network geometry.




Counter anion exchangeMetal-metathesis

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**P-90**

# In Silico Exploration of Thiazolidin-4-one derivatives as Potential wild-type and Double MutantInhibitors of HIV-1 Reverse Transcriptase Enzyme

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Reverse transcriptase (RT) is an initial attractive and crucial key target for the replication of HIV-1 virusand also the development of anti-HIV drugs.The virally encoded reverse transcriptase (RT) enzyme is responsible for the conversion of its single-stranded RNA to double-stranded DNA.Currently, five NNRTIs i.e., nevirapine, delavirdine, efavirenz, etravirine, and rilpivirine have been emerged against the RT for the clinical treatment of AIDS. [1]However, NNRTIstherapy is become inactive against HIV-1 virus multiplication due to developmentof drug resistance. In the present work, we evaluated a set of selected hybrid C-2, N-3 and C-5 modified thiazolidin-4-one analogues to identify potential pharmacophoric features against the wild type and mutant strains by using molecular docking approach. [2] Docking results obtained from the hybrid thiazoldin-4-ones in to the active site of RTby using Molecular Operating Environment (MOE) program indicated that the compounds showed a comparable potency with a retention of activities against the Wild-type and double mutant strains of Tyr181Cys/Lys103Asn, of HIV-1 reverse transcriptase enzymes (Figure 1). [3,4] Among the designed analogues, compounds having mesityl moiety, 3,5-dihalo phenyl at C-2 and biphenyl, 4-cyanophenylamine &1-napthol at N-3of thiazolidin-4-one showed significant binding free energy against wild strain(-8.29, -8.80, -8.74, -8.76 & -8.35 kcal/mol) and against double mutantstrain (-8.64, -8.45, -8.23, -8.22 & -8.20 kcal/mol) of HIV-1 RT, respectively. The molecular insight study of proposed, hybrid thiazoldin-4-ones might be useful in the design of novel RT inhibitors with high ligand efficacy on single and double resistant strains.

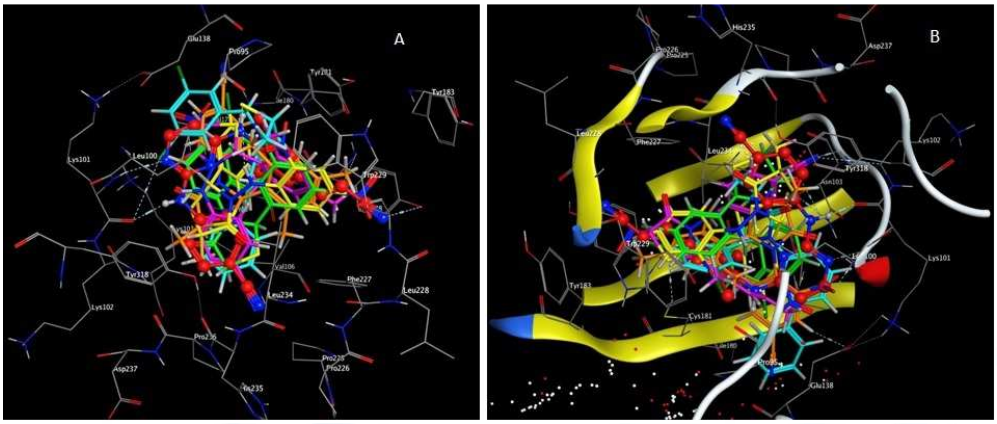


**Figure 1**: Binding pose of selected thiazolidin-4-ones in the active site of Wild-type (A) and Tyr181Cys/Lys103Asn (B) mutant strains of HIV-1 RT

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**P-91**

# Design of Schiff-base Functionalized Imidazolium Ionic Liquid Fluorescent Sensor for $Al^{3+}$ ion

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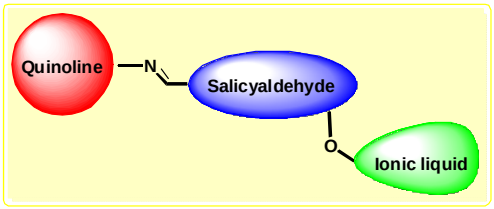
**Abstract:** Functionalized ionic liquids, which are a class of neoteric solvents composed entirely of ions, are drawing extensive interest, since they can be tailored to satisfy the functional requirements for building organic materials by changing either the cation or anion species [1]. Functionalized ionic liquids have achieved great success in acting as luminescent materials, exhibiting strong fluorescence with high quantum yields [2]. Aluminum is the third most abundant of all elements and widely exists in the environment because of acidic rain and human activities. It is a very toxic element as it hampers plant growth and also damages the human nervous system leading tovarious serious diseases viz.Parkinson's and Alzheimer's [3] etc. In recent years, fluorescent chemosensors have attracted significant interest because of their potential applications in medicinal and environmental research. HereinSchiff-base functionalized imidazolium ionic liquid fluorescent sensor for $Al^{3+}$ has been synthesized and characterized (Scheme 1). The addition of $Al^{3+}$ makes significant increase in the fluorescent intensity of sensor in water, however, other metal ions have almost no influence on the fluorescence. Details of synthesis and characterization of sensor along with its metal sensing application will be shown in poster presentation.




**Scheme 1: Sensor architecture**

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P-92

# A BIOPHYSICAL INVESTIGATION OF THE EFFECT OF NON-ENZYMATIC GLYCATION OF HUMANΓB-CRYSTALLIN

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Nonenzymatic glycation is a bimolecular condensation reaction between a reducing sugar and the free amino group of the protein. In the eye protein crystallins, glucose reacts with the ε-$NH_2$ group of lysine residue to form ε-N deoxyfructosyllysine. Cataract is the major cause of impaired vision worldwide, which is eventually associated with conformational changes of ocular lens proteins.Yan*et al.*, Nahomi*et al.*[1,2]It has been reported that diabetic patients often suffer from earlier onset of cataract formation. The key pathogenesis of cataract formation is the greater extent of glycation in eye proteins. Enhanced concentration of glucose in blood leads to several chemo-physical modifications of eye lens protein crystallin. The present study mainly focuses on the *in vitro* glycation of recombinant human γB-crystallin in presence of elevated concentrations of glucose under physiological conditions. Chaudhury*et al.*[3] The glycated protein has been purified by affinity chromatography and the formation of advanced glycation end products (AGEs) has been monitored fluorimetrically. Circular dichroism spectroscopy studies show loss of secondary structure during prolonged glycation. Size exclusion chromatographic studies suggested the formation of covalently linked dimer which was not due to disulfide bond. MALDI-TOF spectroscopy shows the attachment of single glucose moiety upon glycation.

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3. S. Chaudhury, P Ghosh, S Parveen, and S Dasgupta, International Journal of Biological Macromolecules. 96, 2017, 392–402.

**P-93**

# A BIOPHYSICAL INVESTIGATION OF THE EFFECT OF NON-ENZYMATIC GLYCATION OF HUMANγB-CRYSTALLIN

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Nonenzymaticglycation is a bimolecular condensation reaction between a reducing sugar and the free amino group of the protein. In the eye proteincrystallins, glucose reacts with the ε-$NH_2$ group of lysine residue to form ε-N deoxyfructosyllysine. Cataract is the major cause of impaired vision worldwide, which is eventually associated with conformational changes of ocular lens proteins.Yan*et al.*, Nahomi*et al.*[1,2]It has been reported that diabetic patients often suffer from earlier onset of cataract formation. The key pathogenesis of cataract formation is the greater extent of glycationin eye proteins. Enhanced concentration of glucose in blood leads to several chemo-physical modifications of eye lens protein crystallin. The present study mainly focuses on the *in vitro* glycation of recombinant human γB-crystallin in presence of elevated concentrations of glucose under physiological conditions. Chaudhury*et al.*[3] Theglycated protein has been purified by affinity chromatography and the formation of advanced glycation end products (AGEs) has been monitored fluorimetrically. Circular dichroism spectroscopy studies show loss of secondary structure during prolonged glycation. Size exclusion chromatographic studies suggested the formation of covalently linked dimer which was not due to disulfide bond. MALDI-TOF spectroscopy shows the attachment of single glucose moiety upon glycation.

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P-94

# IMPACT OF POLYPHENOLS ON THE AGGREGATION OF LYSOZYME AND RNase A

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Oxidative stress induced protein aggregation is one of the major risk factors for a wide range of chronic, metabolic, and neurodegenerative disorders like Alzheimer's disease, Parkinson's disease etc. Antioxidant therapy is often used to prevent the oxidative damage to proteins. Recently natural polyphenols have received significant interest in the research community because of their ability to suppress oxidative stress. Porat *et al.* [1] In this study, we have investigated the impact of various polyphenols - gallic acid (GA), epicatechin gallate (ECG), and epigallocatechin gallate (EGCG) on the oligomerization of hen egg white lysozyme (HEWL) and ribonuclease A (RNase A) using different biophysical techniques. Results showed that GA inhibited the aggregation of lysozyme in a concentration dependent manner. Electrophoresis and cyclic voltammetry experiments have been performed to explore the mechanism of inhibition that suggested GA covalently binds to the hydrophobic Trp62/Trp63 residues via its quinonic form and restricts their exposure towards solvent under denaturing condition. It has also been revealed that Met residues of HEWL are oxidized to induce more polar environment around the protein. On the other hand, GA and ECG are found to prevent oxidatively imposed dityrosine (DT) cross-linkages in RNase A to a large extent, but they promote protein oligomerization with EGCG because of protein-polyphenol cross-linking. We have further proved that polyphenol/β-cyclodextrin (β-CD) inclusion complexes can efficiently prevent both protein oligomerization and DT formation as the quinone forming ring of polyphenols become encapsulated in the cavity of β-CD and are no longer available for protein cross-linking.

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**P-95**

# Attenuation of arsenic induced ROS, DNA damage in murine derived IEC-6 cell line by Mangiferin: involvement and possible chelate effect

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In natural water bodies contaminated by arsenic poses severe health problems. Arsenic predominantly exists as pentavalent form arsenatein oxidizing ground water conditions and other as trivalent arsenite. Cure for arsenic toxicity remains obscure.Mangiferin a C-glucosyl xanthone was investigated for its ability to protect against arsenic induced cytotoxicity in IEC-6 cell lines. The UV spectral information indicated the chemical interactions between mangiferin and Arsenic in a 4:1 molar ratio. Furthermore the kinetic course of forward as well as reverse titrations showed the interaction of antioxidant and arsenic.MTT assays confirmed the efficacy of MGN supplementation in attenuating arsenic induced cytotoxicity. Mangiferin could effectively attenuate the arsenite-induced cytotoxicity, production of reactive oxygen species (ROS), MMP, lipid peroxidation, DNA damage and cell cycle. Application of mangiferin along with $NaAsO_2$ in IEC-6 cells resulted in the modulation of arsenate-induced activities of antioxidant enzymes like SOD, Catalase and GSH to near normal levels. Migration assay also indicated the wound healing ability of mangiferin in intestinal epithelial cells. FTIR, florescence studies indicated possible chelation of mangiferin with arsenic. We suggest that Mangiferin which bioactive component of *Mangifera indica* ameliorates arsenic induced cytotoxicity and genotoxicity in IEC-6 cell line.

P-96

# Synthesis, crystal structure and biological profile of tailored water soluble Ag(I) nalidixic acid–piperazinium drug candidate: Validation of specific chemotherapeutic potential for MIA-PA-CA-2 cancer cell line

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**Abstract:** Novel ionic Ag(I)−piperazinediium nalidixic acid conjugate (**1**) was designed and synthesized as antitumor chemotherapeutic drug entity and was characterized by elemental analysis, FT−IR, $^{1}H$, $^{13}C$, ESI MS and single crystal X−ray crystallography. Complex**1** resulted from proton transfer reaction between nalidixic acid (HnaI) and piperazine (pipz); and its subsequent complexation with silver nitrate salt. Complex **1** crystallized in triclinic space group *P 1* and comprises of a dipiperazinium silver cationic unit, two nalidixate anionic moieties and a nitrate ion. The silver(I) ion was shown to adopt a linear configuration upon coordination with two nitrogen atoms of piperazine cations arranged in trans fashion. Preliminary *in vitro* interaction study of complex **1** with ct–DNA and tRNA was investigated by electronic UV–vis titrations, fluorescence spectroscopy, circular dichroism, and the mode binding was proposed to be electrostatic. Complex **1** exhibited more avid binding propensity towards RNA which was deduced from its larger $K_b$ and $K$ values. Significant inhibitory effects on the catalytic activity of Topo I enzyme by **1** was observed at **25** μM concentration. An analysis of Hirshfeld surfaces and fingerprint plots were carried out to study the comparison between intermolecular interactions, which are crucial in building different supramolecular architectures involving combinations of N–H…..O, O–H….O and CH…..O linkages into two–dimensional framework. Molecular docking studies of the complex were carried out with DNA, RNA and Topo I targets to ascertain the specific binding mode which further substantiated the spectroscopic results.Cytotoxic studies were carried out on a panel of human cancer cell lines *viz*., MIA-PA-CA-2, HepG2, HeLa and MCF7 by SRB assay which revealed significant regression selectively for MIA–PA–CA–2 cancer cell line ($GI_{50}$ value < 10).

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P-97

# Vancomycin loaded pH-responsive chitosan nanoparticles as a nanoantibiotic against methicillin-resistant *Staphylococcus aureus*

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**Purpose:**
The design and synthesis of novel pH-responsive nanoantibiotics is an emerging new research areato address the antibiotic resistance crisis [1,2]. Therefore, the purpose of thisstudy was to synthesize a new anionic gemini surfactant (AGS) for the formulation of pH-responsive chitosannanoparticles(CSNPs) to treat methicillin-resistant *Staphylococcus aureus* (MRSA) infections.

**Methods and Materials:**
The coupling of oleic acid with 2,2-dimethyl-5,5-bis(hydroxymethyl)-1,3-dioxane and subsequent deprotectionfollowed by reaction with succinic anhydride and sodium bicarbonate yielded the AGS. Critical micelle concentration (CMC) was determined using conductometryandin vitro cytotoxicity was performed on Hep G2 cells.Vancomycin loaded CSNPs containing AGS were prepared by ionotropic gelation of chitosan with pentasodiumtripolyphosphate. CSNPs were characterized for size, polydispersity index (PDI), zeta potential (ZP), entrapment efficiency, surface morphology, in vitro drug release and in vitro antibacterial activity (at pH 6.5 and 7.4). The results of in vitro antibacterial activity were further supported by in vivo study using a mice skin infection model.

**Results:**
The structure of AGS was confirmed by FT-IR, NMR and MS and its CMC was found to be 1.3 mM/L. AGS was non-toxic as percentage cell viability of Hep G2 cells was >85% at all tested concentrations. The CSSNPs were spherical with size, PDI and ZP of 220.57±5.9 nm, 0.299±0.004 and 21.9±0.9 mV respectively. The increased and controlled release of vancomycin was observed at acidic pH (6.5) compared to neutral pH (7.4).The minimum inhibitory concentration values at pH 6.5 and 7.4 against MRSA were 7.81 and 62.5 µg/mL.The mechanism involved could be a decrease in ionization of AGS under mildly acidic conditions resulting into destabilization of the CSNP structure and release of more vancomycin. In vivo antibacterial activity performed on BALB/c mice showed that CSSNPs reduced the MRSA count by almost 8-fold in animals treated with vancomycin loaded CSSNPs compared to those treated with plain vancomycin.

**Conclusion:**
A pH-responsive nanoantibiotic developed in this study confirms its potential for targeted delivery of antibiotics to infection siteto control MRSA infections.

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**P-98**

# *In vitro* anti-arthritic activity and phyto-chemical profiling of marine brown algae *Sargassum ilicifolium*

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**ABSTRACT:** With marine species comprising approximately a half of the total biodiversity of the earth, the sea provides enormous novel compounds and it is classified as the natural bioactive reservoir that can be explored for drug activity. The macro algae occupy a potentially important place as a source of biomedical compounds. In the present study, *invitro* anti-arthritic activity of the aqueous extract of the seaweed *Sargassum ilicifolium* was investigated by protein denaturation method by using bovine serum albumin. The investigation is based on the need for newer anti-inflammatory agents from natural source with potent activity and lesser side effects as substitutes for chemical therapeutics. Anti- denaturation study is performed. The production of auto antigen in certain arthritic disease may be due to denaturation of protein. Phytochemical profiling was carried out for the aqueous extract using Gas chromatography-Mass Spectroscopy. The brown algae *Sargassum ilicifolium* was collected from Mandapam area, Rameshwaram, authenticated, washed, shade dried and the aqueous extract was prepared by maceration, concentrated, dried and used to test Anti-arthritic activity. From the results, it can be stated that aqueous extract of *Sargassum ilicifolium* (82.67%) are capable of controlling and inhibiting denaturation of protein comparable with that of Diclofenac sodium (91.83%). GCMS analysis of aqueous extract of *Sargassum ilicifolium* revealed the presence of bioactive principles like zingerone, n-Hexadecanoic acid, 9H-Cycloisolongifolene-8 oxo- 9,12-Octadecadienoic acid, Stigmasterol, β-sitosterol. Therefore, our study support the use of active constituents from *Sargassum ilicifolium* in treating inflammation and it might be helpful in preventing or slowing the progress of various inflammatory disease.

**Keywords***:* *Sargassum ilicifolium*, Protein denaturation, Anti-arthritic activity, GC-MS.

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**P-99**

# INHIBITION OF AMYLOID BETA PEPTIDE AGGREGATION BY FULLERENE AND ITS CONJUGATES: A MOLECULAR DOCKING APPROACH

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Alzheimer's disease is induced upon chronic imbalance of production and clearance of amyloid beta (Aβ) peptides (39-43 residues) and consequent *in vivo* aggregation into highly ordered fibrils. These fibrils deposit as insoluble plaques in the brain vasculature and parenchyma. The $A\beta_{25-35}$ fragment is the most toxic fragment of the full length peptide and undergoes very rapid fibrillation. Fullerenes have displayed inhibition of Aβ aggregation in vitro, with high specificity towards the KLVFF recognition motif (Lee *et al*., [1]), and have recently captured attention because of their strong hydrophobicity and large surface area. We have used molecular docking (AutodockVina) to investigate the interaction of fullerenes of varied sizes with $A\beta_{25-35}$, $A\beta_{1-42}$ and $A\beta_{9-40}$ (β-sheet). High negative binding energy values indicate favorable hydrophobic interactions between fullerenes and all three peptide sequences, with minimum energy values for fullerenes with 60-70 carbon atoms. *ΔASA* calculations have shown that the binding residues get more shielded with increase in size of the fullerenes. We have designed various novel conjugates of $C_{60}$ fullerene with peptide analogues of KLVFF and LPFFD sequences and surfactants (SDS, CTAB), with linkages based on various reported fullerenyl amino acids and peptides. Docking studies have shown that the fullerene linked ligands show better interactions with single Aβ peptide and Aβ sheet than free fullerene and free peptide analogues and surfactants. The interacting residues are mainly those which are involved in the formation of β-sheet rich oligomers. Hence functionalized fullerenes can act as potential therapeutic agents by obstructing or destabilizing β-sheet formation.

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**P-100**

# Synthesis, Characterization and Biological Evaluationof Reactive Dyes Based on 5-(4-chlorophenyl)-1,3,4-thiadiazole-2-amineand Their Dyeing Performance on Various Fibres

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**ABSTRACT:** A series of reactive dyes has been synthesized by diazotization of 5-(4-chlorophenyl)-1,3,4-thiadiazole-2-amine and coupled with 1-phenyl-3-methyl-5-amino pyrazole. Maradiya[1]; C Reddy et al.[2], SJadhav et al.[3]. The resulting compound was further diazotized and coupled with various cyanurated acids to give Reactive Dyes. The Synthesized reactive dyes were characterized by the UV-Visible, IR &$^{1}$H NMR. Their dyeing performance on silk, wool and cotton has been assessed. The percentage dye bath exhaustion on different fibres was reasonably good and acceptable. The dyed fibres showed moderate to very good fastness to light, washing and rubbing. Furthermore the antimicrobial activities of synthesized dyes were assessed and found to be moderate to good.

**KEYWORDS:** pyrazole, thiadiazole, diazotization, Antimicrobial activity.

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**P-101**

# SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL EVALUATION OF SOME PYRAZOLE BASED CHROMENOPYRIMIDINE DERIVATIVES

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**ABSTRACT:** A new series of chromenopyrimidine N-(4-(5-(substitutedphenyl)-4,5-dihydro-1H-pyrazol-3-yl)phenyl)-5H-chromeno[2,3-d]pyrimidin-4-amine Mobinikhalediet al. [1] have been synthesized from 1-(4-(5H-chromeno[2,3-*d*]pyrimidin-4-ylamino)phenyl)-3-(substitutedphenyl)prop-2-en-1-one. They were characterized by elemental analysis, IR and PMR spectroscopy. The newly synthesized compounds were screened for their antimicrobial activityAmatur et al. [2]. Some of the compounds showed moderate to significant activities.

**KEY WORDS:** chromenopyrimidine, pyrazole, antimicrobial

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**P-102**

# Synthesis of biologically active methylene derivatives of Thiazolidinone

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**ABSTRACT:** A series of3,3'-(4,4'-methylene bis(2,5-difluoro-4,1-phenylene))bis(2-substituted phenylthiazolidin-4-one) were synthesized frombis *N*-Mannich base and tested for their antibacterial, antifungal and antiviral activities.N. Desai et al. [1]; C. Alessia et al. [2] Most of the compounds showed moderate-to-significant antibacterial and antifungal activities. The compounds did not show selective activity against HIV. Some of the compounds have been evaluated for anticancer activity, but they were found as poorly active. The structures of the synthesized compounds were elucidated by IR and $^{1}$H NMR spectroscopy.

**KEYWORDS:** Thiazolidin, Methylene, Mannich base.

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P-103

# Synthesis and Biological Evaluation of Some Reactive Dyes having 4(3*H*)-quinazolinone Molecule for the Dyeing of Silk, Wool and Cotton Fibres

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**ABSTRACT:** The objective of the current study was to introduce the quinazolinone molecule into a conventional reactive dye system. On this basis, twelve quinazolinone based dichloro-s-triazine reactive dyes($D_1$-$D_{12}$) were rapidly and efficiently synthesized by coupling route of diazotized 3-(6-amino-1,3-benzothiazole-2-yl)-2-phenylquinazolin-4(3*H*)-one with a variety of cyanurated coupling components Patel et al.[1]; Parekh et al[2]. Their characterization was done using elemental analysis, UV Vis, IR, $^1$H NMR spectroscopy. Their dyeing performance as reactive dyes have been assessed on silk, wool and cotton fabrics. The percentage dye bath exhaustion and fixation on different fibres were found to be very good. The dyed fabric showed moderate to very good light fastness and good to excellent washing and rubbing fastness properties. Spectral properties and colorimetric data of synthesized dyes have also been studied in detail. Furthermore the antimicrobial activities of synthesized dyes were assessed and found to be moderate to good.

**KEYWORDS:** 4(3*H*)-quinazolinone, Exhaustion, Fixation, Fastness Properties, Colorimetric Data, Antimicrobial activity.

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**P-104**

# Synthesis, characterization and antimicrobial activity of Schiff base containing thieno[2,3-*d*]pyrimidine moiety

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**ABSTRACT:** Thienopyrimidine derivatives, which are structure analogues of purines, have been focus of great interest because of their large range of pharmacological activities Rashad et al[1]. Numerous thieno[2,3-*d*]pyrimidines have been proved useful for cerebral ischemia, tuberculosis, Alzheimer's and Parkinson's diseases Zhu et al[2]. In an effort to synthesize antimicrobial agents, we report herein the synthesis of *a* newseries of Schiff bases ofthieno[2,3-*d*] pyrimidine*N*-(4-((Substitutedbenzylidene)amino)phenyl)-5,6,7,8-tetra hydrobenzo[4,5]thieno[2,3-*d*]pyrimidin-4-amine($A_1$-$A_{10}$)were synthesized fromEthyl 2-amino-4,5,6,7-tetrahydro-1-benzothiophene- 3-carboxylate as a key intermediate. The characterization of the newly synthesized compounds was established by IR, $^1$H NMR and elemental analysis. The synthesized compounds were screened for their antibacterial activity against *S.aureus* and *S.pyogenes*fromGram-positivegroup of bacteria and*E.coli* and *P.aeruginosa*from Gram-negative group of bacteria and antifungal activity against *C.albicans*, *A.niger*and*A. clavatus*.

**KEYWORDS:** Thieno[2,3-*d*]pyrimidine, Schiff's base, Antibacterial Activity, Antifungal Activity.

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**P-105**

# Synthesis and Characterization of some Thiazolidinone derivatives containing Mannich base of Sydnone as antimicrobial agents

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**ABSTRACT:** A new series of 4-((4-(2-(substitutedphenyl)-4-oxothiazolidin-3-yl)phenylamino)methyl)-3-(3-nitrophenyl)-sydnone have been synthesized from 4-((4-(substitutedbenzylideneamino)phenylamino)methyl)-3-(3-nitrophenyl)-sydnone. They were characterized by elemental analysis, IR and $^{1}$H NMR spectroscopy. The newly synthesized compounds were screened for their antimicrobialOmar et al.[1];Vicini et al.[2]activity. Some of the compounds showed moderate to significant activities.

**KEY WORDS:** sydnone, thizolidinone, antimicrobial

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P-106

# DESIGN, SYNTHESIS AND ANTIMICROBIAL ACTIVITY OF NOVEL QUINOLINE DERIVATIVES ENCOMPASSING PYRAZOLINE AND PYRIDINE SCAFFOLDS

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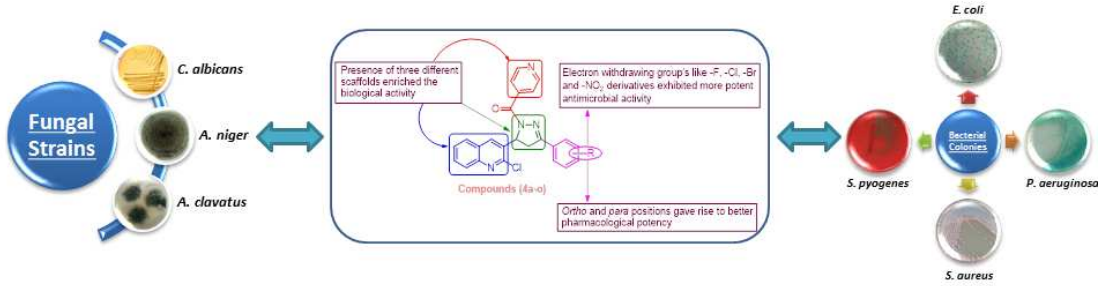
The present investigation is in the interest of some synthesized novel derivatives containing (3-(2-chloroquinolin-3-yl)-5-(aryl)-4,5-dihydro-1*H*-pyrazol-1-yl)(pyridin-4-yl)methanones (**4a-o**) moieties incorporated with different biological active heterocycles such as quinoline, pyrazoline and pyridine derivatives. For the determination of the compounds reported in this paper was based on FTIR, $^{1}$H NMR, $^{13}$C NMR and mass spectral data and same compounds were screened for their antibacterial and antifungal activity on four bacteria (*S. aureus*, *S.* pyogenes, *E. coli*, *P. aeruginosa*) and three fungi (*C. albicans*, *A. niger*, *A. clavatus*) using ampicillin and griseofulvin as the standard drugs. Cytotoxicity study was carried out using MTT colorimetric assay (HeLa cell line). Among the screened compounds, **4e**, **4f** and **4n** showed most potent antibacterial activity, while compounds **4d** and **4g** emerged as the most active against fungal strains. The results demonstrated that compound **4o** was remarkably active against all microbial strains. From the viewpoint of SAR studies, it was observed that the presence of electron withdrawing groups remarkably enhanced the antimicrobial activity of synthesized compounds. Additionally, preliminary MTT cytotoxicity studies on HeLa cells suggested that effective antimicrobial activity of **4e-g**, **4n** and **4o** was accompanied by low cytotoxicity.



P-107

# Pyrazole, 1,3,4-oxadiazole and pyridine as ubiquitous structural fragments in heterocyclic chemistry

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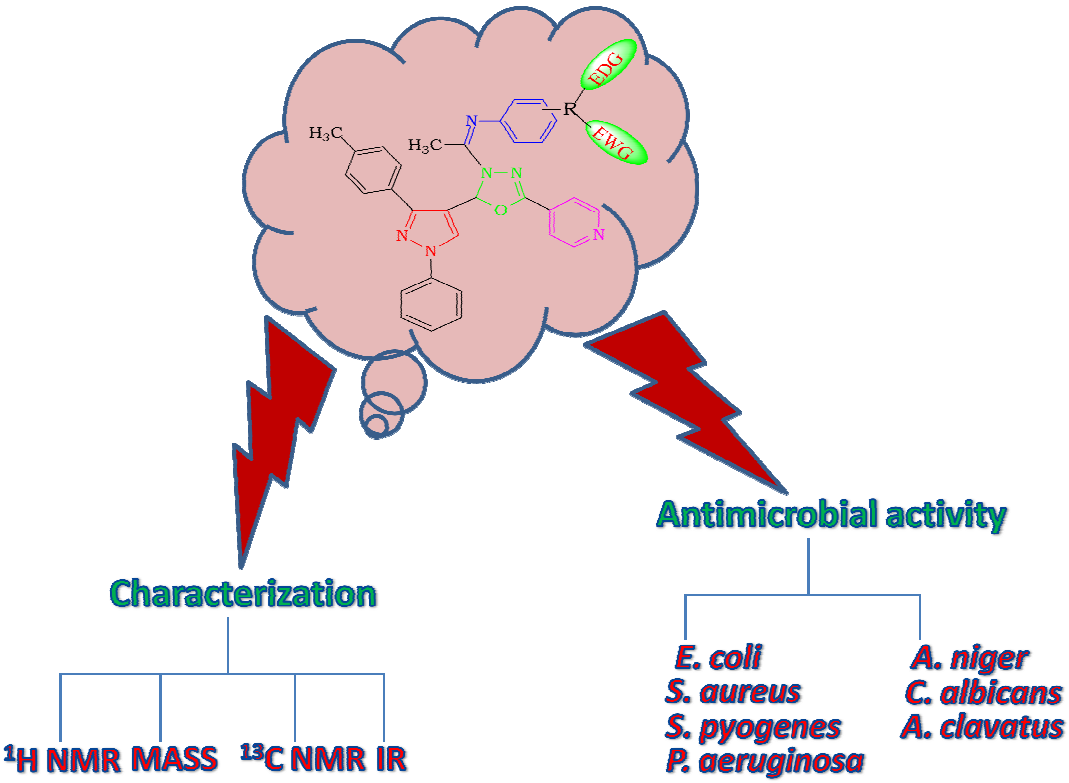


**Abstract:** Nitrogen-rich heterocycles, particularly pyrazole 1,3,4-oxadiazole and pyridine, represent an exclusive Class of diversified frameworks exhibiting a broad spectrum of biological functions. We synthesized novel series of*N*-(1-(2-(1-phenyl-3-(p-tolyl)-1*H*-pyrazol-4-yl)-5-(pyridin-4-yl)-1,3,4-oxadiazol-3(2*H*)-yl)ethylidene)arylanilineand their derivatives. The chemical structures of synthesized compounds were characterized by physicochemical and analytical methods ($^{1}$H NMR, $^{13}$C NMR, IR and Mass spectroscopic methods).Synthesizedderivatives evaluated their antimicrobial activity against responsible bacteria such as, *E. coli*, *P. aeruginosa*, *S. aureus* and *S. pyogenes* and responsible fungi such as, *C. albicans*, *A. niger* and *A. clavatus.*

P-108

# NOVEL AND CONVENIENT SYNTHESIS OF 4-THIAZOLIDINONEINCORPORATED QUINOLONES DERIVATIVES AS ANTIMICROBIAL AGENTS

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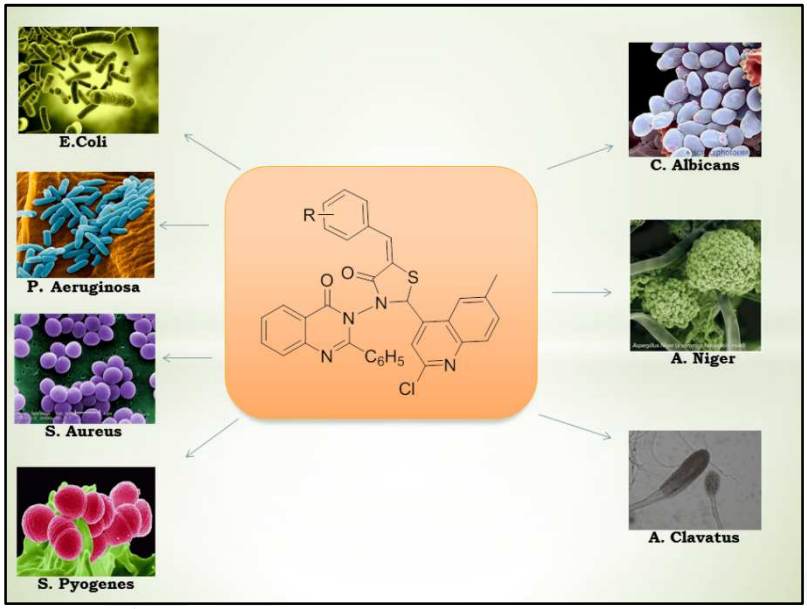
The age old drug therapy found to be ineffective against drug-resistant microbial pathogens and has lent additional urgency in microbiological research.In continuation to this, the synthesis of novel series of structurally related 4-thiazolidinone and quinolones derivatives is described.A series of novel 5-arylidene-2-(2-chloro-6-methylquinolin-4-yl)-3-(4-oxo-2-phenylquinazolin-3(4*H*)-yl)thiazolidin-4-ones were designed containing significant pharmacophoric features.Newly synthesized scaffolds were interpreted with the use of different analytical techniques likeFTIR, $^{1}$H-NMR, $^{13}$C-NMR and mass spectrometry. Their biological activity against various bacteria and fungi species was investigated.Antimicrobial activity was measured against *Staphylococcus aureus* (MTCC 96), *Candida albicans* (MTCC 227), *Aspergillus niger* (MTCC 282), Streptococcus pyogenes (MTCC 442), *Escherichia coli* (MTCC 443), *Aspergillus clavatus* (MTCC 1323) and *Pseudomonas aeruginosa* (MTCC 1688) by serial broth dilution method.The antimicrobial screening data revealed that selected screened compounds exhibited significant activity against all microbial and fungal strains.



P-109

# Evaluation and assessment of baseline heavy metals contamination in marine water and sediment samples from the along coast of South Gujarat estuarine regions-west coast of India

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**Abstract:** Encroachment, disposal of untreated domestic and industrial water and dumping of solid wastes have degrade the overall quality of the estuarine regions at coast of south Gujarat region. The present study investigated seasonal and the extend of pollution of marine water and sediment of these estuaries and analyzed the regional variability of the concentration of Cr, Pb, Ni, Cu, Mn and Cd-all of concern because of their potential toxicity, using atomic absorption spectrophotometer as per US EPA sediment quality guideline.

Some other pollution indicator parameters like pH, DO, BOD, and organic matter were investigated. Samples collected and analyzed during (i) summer (ii) monsoon and (iii) winter seasons in theyear of May 2015 to March 2016.

The study area covered eight estuaries of south Gujarat like Veroni, Damangnaga, Kolak, Par, Auranga, Ambica, Purna and Mindhola out of this eight estuariesDamangang, Kalak, Par, and Mindhola estuaries were more polluted than other estuaries.

Heavy metals data suggested that there is a serious threat to marine flora-fauna from high concentration of metals. The study also demonstrates a threat to both terrestrial and aquatic ecosystem. The results suggested that they can be used as baseline data for heavy metals and other parameters and also suggest that enrichment of heavy metals due to rapid industrialization and anthropogenic activities in this region.

**P-110**

# Oxazine bearing pyridine scaffolds as potential antimicrobial agents

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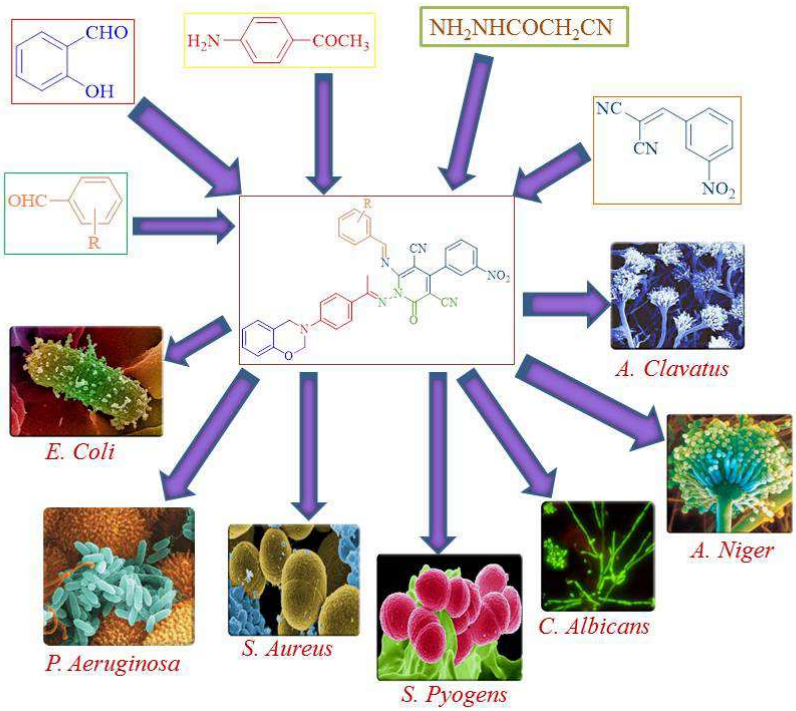
**Abstract:** A series of novel compounds 1-((1-(4-(2*H*-benzo[e][1,3]oxazin-3(4*H*)-yl)phenyl)ethylidene)amino)-6-((benzylidene)amino)-4-(3-nitrophenyl)-2-oxo-1,2-dihydropyridine-3,5-dicarbonitrile**(7a–o)** were synthesized by a sequence of multistep reactions. Structure confirmation of newly synthesized compounds has been performed by $^{1}$H NMR, $^{13}$C NMR, IR and mass spectral data. Antimicrobial activity of the titled compounds **(7a–o)** was studied against two strains of Gram-positive bacteria (*Staphylococcus aureus* and *Streptococcus pyogenes*), two strains of Gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*) and three strains of fungi (*Candida albicans, Aspergillus niger*and *Aspergillus clavatus*) by serial dilution method. Compounds **7f** and **7k** exhibited significant antimicrobial activity.



**P-111**

# Synthesis and antimicrobial evaluation of some new 1,3,4- oxadiazoles

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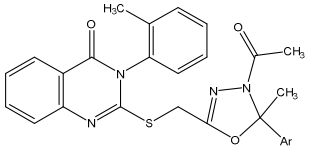
**ABSTRACT:** Recently the investigations in the field of oxadiazole have intensified due to the large number of uses of oxadiazoles in the most diverse areas, 1,3,4- oxadiazole derivatives have been reported to show biological activities like bactericide[1] and fungicide [2]properties. These observations and our previous work [3]of oxadiazole prompted us to synthesize unreported derivatives of 1,3,4- oxadiazole. A series of 2-((4-acetyl-5-(aryl)-5-methyl-4,5-dihydro-1,3,4-oxadiazol-2-yl)methylthio)-3-o-tolylquinazolin-4(3H)-one was synthesized by the cyclization of imines using acetic anhydride. The Schiff base are obtained by the reaction of appropriate carbonyl compound with 2-(4-oxo-3-o-tolyl-3,4-dihydroquinazolin-2-ylthio) acetohydrazide. The structure of synthesized compounds was characterized by IR, $^{1}$H-NMR, $^{13}$C-NMR and mass spectrometry. The synthesized compounds were screened for their antimicrobial activity against different strains of Gram-negative (*E. coli* and *P. aeruginosa*) and Gram-positive (*S. aureus* and *S. pyogenus*) bacteria and selected fungi*C. albicans, A. niger* and *A. clavatus* using serial broth dilution method. Our approach is to focus on the modification of synthetic pathway for the said reaction with respect to time and other physico-chemical parameters.




Where, Ar = Differnt aryl groups

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P-112

# Antimicrobial activity of hydrophobhic peptide derived from IL-8 of a teleost

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**ABSTRACT:** Chemokine plays an important role during inflammatory response in humans and other vertebrate organisms.Interleukin 8 (IL-8) is a member of CXC chemokine family and a chemoattractant cytokine produced by variety of tissues and blood cells.They act as a viaduct between innate and adaptive immune system in fish. In this study, we have identified a CXC chemokine from the cDNA library of *Channa straitus*(*Cst*), a freshwater teleost.The CstIL-8 cDNA was 291 basepairs in length with an open reading frame of 97 amino acids. We describedthe antimicrobial features of cationic peptide namely WS12($^{85}$WVKKVIQRIMSS$^{96}$) derived from C-terminal of the *Cst*IL-8 protein.Structural analysis of the peptide was showed that hydrophobic face and cationic rich amino acids are present on either side of the helical wheel. The disc diffusion assay exposed that the peptide WS12 had bactericidal activity against *Salmonella enterica*, *Escherichia coli*, *Bacillus cereus*,*Bacillus mycoides*,*Vibrio harveyi* and *Serratia marcescens*. The peptide WS12 showed significant zone of inhibition against gram positive bacteria*B. cereus* (15±1 mm). Minimum inhibitory concentration assay was showed that the peptide WS12 had complete bactericidal activity at concentration of 25 µM against *B. cereus*. Flow cytometric analysis revealed that the 40% of *B. cereus* cells stained with propidium iodide, upon treatment with WS12 at the concentration of 25 µM/mL. Hence, WS12 peptide seems to have its antimicrobial activity against *B. cereus*through membrane disruption.The peptide WS12 has no cytotoxic activity towards fish leucocytes at the concentration of (25 µM). Additionally, scanning electron microscope (SEM) observation confirmed that WS12 peptide treatment completely damaged and destructed *B. cereus* cells. Taken together, these findings suggest that WS12 peptide would be a safe and potential therapeutic molecule substitute to antibiotics in various clinical fields.

**P-113**

## Insights into the bactericidal role of carbohydrate recognition domain of fish lectin

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Antimicrobial peptides (AMPs) are small innate immune proteins that are found in wide variety of species. They are involved in various biological functions such as apoptosis, wound healing and immune modulation. Lectins are a group of sugar binding proteins that specifically recognize sugar complexes. They possess the ability to agglutinate erythrocytes with known carbohydrate which have one non-catalytic domain that binds reversibly to specific monosaccharide or oligosaccharides. In terms of drug delivery, the carbohydrate mediated biorecognition of lectins resulting in mucoadhesion, cytoadhesion and cytoinvasion might be advantageous for drug delivery to the small intestine. Here we report a full length lily type lectin -2 (LTL-2) identified from the cDNA library of snakehead murrel *Channa striatus*. *Cs*LTL-2 protein contains a B-lectin along with three carbohydrate binding sites which is prominent characteristic functional feature of LTL. To evaluate the antimicrobial property of *Cs*LTL-2, the carbohydrate recognition domain was synthesized as short peptide (QP13); and its bactericidal property was analyzed. In addition, QP13 was labeled with fluorescein isothiocyanate (FITC) and its binding affinity with the bacterial cell membrane was analyzed. Minimum inhibitory concentration assay revealed that QP13 inhibited the growth of *Escherichia coli* at a concentration of 80µm/ml. Confocal microscopy imaging showed that QP13 reduced the bacterial cell count drastically. Therefore, the mechanism of action of QP13 on *E. coli* was determined by propidium iodide internalization assay which confirmed that QP13 induced bacterial membrane disruption. Moreover the peptide did not show any cytotoxity towards fish peripheral blood leucocytes. From the results, it was noticed that the QP13 derived from *Cs*LTL-2 plays a significant role in antimicrobial property against the tested pathogens which may find applications in many therapeutic areas.

P-114

# Studies on Interacting Blends of s-triazine-epoxy residue containing unsaturated polyesters and methamethacrylate monomer

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**ABSTRACT:** Novel acrylated unsaturated polyesters (PEs) were prepared by reaction of various 4, 4'-(6-piperazine-1,3,5-triazine-2,4-diyl)bis(oxy)dibenzoic acids(1a-c) with epoxy resin of bisphenol-A using a base catalyst. The post reaction of each of this PEs was carried out with acryloyl chloride V Thulasiraman et al[1]. The resultant products are designated as acrylated polyesters (APEs). The PEs and APEs were characterized by elemental analysis and IR spectra of PEs and APEs were also recorded. Blending of these APEs were carried out with methyl acrylate monomer V Shukla[2]. The curing of these APEs-Methyl acrylate blends was monitored on a differential scanning calorimeter (DSC) by using benzoyl peroxide as a catalyst. Based on DSC data, the glass fiber reinforced composites of APEs-Methyl acrylate blends have been fabricated and their chemical, mechanical and electrical properties have been evaluated. The unreinforced cured samples of APEs-Methyl acrylate blends were analyzed thermogravimetrically.

**KEYWORDS:** Epoxy resin (DGEBA), Polyester, Number average molecular weight, Differential scanning calorimeter (DSC), Thermogravimetric analysis (TGA), Interacting blends.

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**P-115**

# Synthesis and antimicrobial activity of thieno[2,3-*d*] pyrimidine moiety

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**ABSTRACT:** A new series of thieno[2,3-*d*] pyrimidine derivatives were synthesized and characterized by elemental analysis, IR, $^{1}$H NMR, $^{13}$C NMR and Mass Spectra. The newly synthesized compounds were screened for their antifungal activity and antibacterial activity against some Gram-positive bacteria and Gram-negative bacteria.[1,2]

**KEYWORDS:** Thieno[2,3-*d*]pyrimidine, Antibacterial Activity, Antifungal Activity

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P-116

# TRANSDERMAL PATCHES OF POORLY SOLUBLE ANTI-HYPERTENSIVE DRUG: FABRICATION & CHARACTERIZATION

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Felodipine, a BCS class II calcium channel blocker, is used in the management of hypertension and angina pectoris. Due to the poor solubility and low bio availability of the drug, there is a necessity to design an alternative route to achieve constant plasma concentration of felodipine for its maximum therapeutic utility and can be achieved by transdermal route.In this study, matrix type transdermal patches were prepared using different combinations of hydrophilic polymer *viz*polyvinyl pyrrolidone (PVP) and hydrophobic polymer *viz*ethyl cellulose (EC) by solvent evaporation technique and were subjected for characterization.The FTIR studies confirmed the compatibility between drug and polymers.Hydrophilic nature of the polymers greatly influenced physical characteristics and dissolution rate.Equal percentage of PVP and EC yielded patches with good folding endurance. The concentration of plasticizer present in the patches gave them desired folding endurance and it increased with the presence of hydrophilic polymer.The formulation with highest PVP concentration, F3, exhibited a maximum drug release of 96.23% for 24 hours. While the formulation with highest EC concentration, F5, exhibited only 74.45% drug release for 24 hours.From the data, formulation F2 (PVP/EC, 2:1) can be concluded as best formulation due to its desired physical characteristics, good initial drug release, sustained release behavior and good *in vitro* permeation. This formulation can be further studied in clinical scenario.

**Keywords:** Calcium channel blocker, Felodipine, Transdermal, Permeation.

P-117

# SOLID DISPERSION OF FELODIPINE FOR IMPROVING RATE OF DISSOLUTION

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**ABSTRACT:** Felodipine, BCS class II calcium channel blocker, is used in the treatment of hypertension and cardiac disorders. Low solubility of felodipine limits its bioavailability. The present study was carried to enhance the dissolution rate of the drug by solid dispersion technology. The solid dispersions were prepared by hot melt technique using PEG4000, PEG6000 and Poloxamer as carriers. The compatibility of the drug and polymers used was confirmed with FT-IR studies. The soliddispersions were prepared in 1:3 and 1:5 drug to polymer ratio. The prepared solid dispersions were analyzed for physical state, X-ray diffraction studies and scanning electron microscopy. The X-ray diffraction pattern of pure drug showed sharp intense peaks which is reduced in the solid dispersions confirming that the drug has changed from crystalline to amorphous form. The SEM images revealed that the drug and the carriers were homogenously mixed and devoid of crystalline particles.The dissolution studies revealed that all the solid dispersions showed an increased dissolution rate when compared to pure felodipine. The dissolution rate increased with an increase in the concentration of carrier molecule. Among the carrier molecules, poloxamer 407 showed highest dissolution rate. The tablets were formulated using poloxamer 407 solid dispersions. The results exhibited that poloxamer 407 SD based tablets gave a significantly higher release of felodipine when compared with control tablets.

**Key words:** Calcium channel blocker, Dissolution, Felodipine, Solid dispersion.

**P-118**

# pH SENSITIVE NANOPARTICLES OF CAPECITABINE FOR TARGETED DRUG DELIVERY

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**ABSTRACT:** In majority cases conventional chemotherapy is leading to discontinuation of therapy due to severe side effects. Chitosan nanoparticles (CsNPs) have gained attention because of their outstanding physical and biological properties and considered as successful candidate for the controlled and targeted anticancer effect by their pH dependent drug releasing ability.Capecitabine (CTB) is widely used as major therapeutic agent for treating breast cancer, however its clinical efficiency in compromised by undesirable side effects coupled with resistance in cancer cells. CTB is incorporated in CsNPs by ionic gelation, with a specific aim to target CTB for site specific delivery. The aim of this study was to assess the feasibility of employing a novel formulation to encapsulate an anionic model drug Capecitabine into chitosan(Cs)-glutaraldehyde nanoparticles(NPs) for site specific delivery. The responses investigated were the entrapment efficiency, mean hydrodynamic particle size andzetapotential. Infrared spectral studies revealed that the drug and polymer are compatible. Four formulations were prepared by varying concentrations of chitosan and glutaraldehyde. All the formulations exhibited nearly same entrapment efficiency, but particle size varied significantly with a change in concentration of formulation variables. At low concentration of chitosan, low particle size was seen whereas, at high concentration of crosslinking agent may resulted increased crosslinking and particle size of 380nm. Among the formulationF2 exhibiteda sustained drug release of 73% due to increased chitosan concentration.

**Keywords:** Capecitabine, Chitosan, Nanoparticles, Tumor-targeting.

P-119

# OPTIMISED LABORATORY SCALE SYNTHESIS OF (2,5-DIOXO-4-IMIDAZOLIDINYL) UREA USING MINERAL ACID AS A CATALYST

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**ABSTRACT:** Dioxo-4-imidazolidinylurea are important scaffolds exhibiting wide therapeutic applications including wound healing, cells regeneration and also useful in cosmetics for itskeratolytic effect[1]. Earlier Lixiu Liu et al. [2] has reported$La_2O_3$-$SiO_2$-$ZrO_2$catalysed synthesis of Dioxo-4imidazolidinyl moiety. However this method has several disadvantages. Therefore a facile method is highly requisite. In this study we develop a new facile mineral acid catalysed protocol for the synthesis of (2,5-Dioxo-4-imidazolidinyl)urea using precursors like oxoethanoic acid and carbonyldiamine in presence of heterogeneous catalyst. We found that this method is general and provided very good yield of the desiredpharamacophoreDioxo-4-imidazolidinyl urea. The characterization of the synthesized derivatives has been carried out by elemental analysis and spectroscopic methods.

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**P-120**

# GC-MS Analysis and Antimicrobial Activity of an Anti-dandruff botanical: *Brassica juncea*

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Indian mustard (Brassica juncea) popularly known as Rai, is one of the most important oilseed crop of Brassicaceae (cruciferous) family. A paste of Rai and Buchanania lanzan is topically applied on the head to prevent dandruff. In view of our interest in antidandruff botanicals we have analyzed its seed extracts using Gas Chromatography–Mass Spectrometry and screened it for its antimicrobial activity. GC-MS analysis of the petroleum ether extract revealed the presence of 38 compounds. (2Z, 13E)-2, 13-Octadecadien-1-ol, hexadecanoic acid, cis-.beta.-farnesene, 3[(trimethylsilyl)oxy]cholest-5-ene, 1H-benzocycloheptene, 2,4a,5,6,7,8-hexahydro-3,5,5,9-tetramethyl-, (R)-, ergost-5-en-3beta-ol, n-tetra tetracontane and n-tetracontane were identified as major compounds. The results of the antimicrobial study suggested that ethyl acetate extract exhibits maximum antimicrobial inhibition activity against tested bacteria Escherichia coli, Staphylococcus aureus and fungus Malassezia furfur. Pet-ether extract of the plant showed moderate antifungal activity, while ethyl acetate, ethanol, and methanol extracts showed significant activity against Candida albicans.

**P-121**

# Synthesis of Hydroxamic Acidsusing Imidazolium Salt Supported *N*-Hydroxy-sulphonamide

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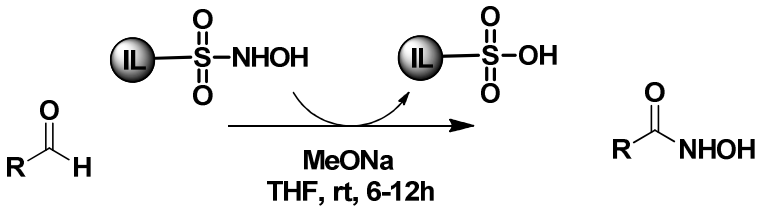
The hydroxamic acid functionality is present in several natural products, drugs (e.g. Vorinostat) and in metal ion chelators [1]. Compounds containing hydroxamic acid functionalityhave shown broad array of biological activities such as antibacterial, antifungal, anti-inflammatry, anti-asthmatic properties[2]. They are generally synthesized from activated carboxylic acids (esters, anhydrides and acid chlorides etc.) and protected/unprotected hydroxyl amines.They can also be synthesized from aldehyde using *N*-hydroxybenzenesulphonamide[3]. Some of these methods suffer from disadvantages such as requirementof removal of side product, product purification, protection and deprotection of hydroxyl amine and preparation of special linker in case of solid phase synthesis. With our interest in exploring application of ionic liquids in organic synthesis, we envisioned that imidazoliumsalt supported N-hydroxysulfonamide can be utilized for the synthesis of hydroxamic acids from aldehydes and some of the issues in their preparation such as removal of side products and purification can be resolved (Scheme 1).In the poster, protocol for the synthesis of imidazoliumsalt supported N-hydroxysulfonamide and its application in synthesis of hydroxamic acids from aldehydes will be presented.




**Scheme 1:** Synthesis of hydroxamic acids using imidazoliumsalt supported N-hydroxy-sulfonamide

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P-122

# Synthesis of Unsymmetrical Sulfides Using Sulfonyl Hydrazide as Thiol Surrogate

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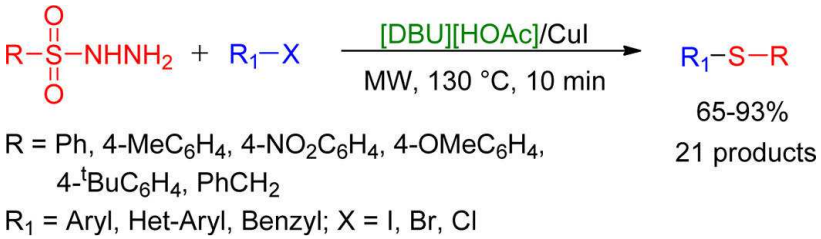
One of the current challenges in organic synthesis is to develop novel, convenient, selective and energy-efficient synthetic methods. As a part of this preoccupation, the search for more practical and environmentally benign synthetic methodologies is of crucial importance.[1] Sulfur-containing organic compounds particularly aryl sulfides and their derivatives are important motifs and powerful molecules having biological, pharmaceutical, and material interest.[2] A number of drugs in therapeutic areas such as diabetes, inflammatory, Alzheimer's, Parkinson's, cancer, and HIV diseases, are found to possess the aryl sulfide fragment. Carbon-sulfur (C-S) bond forming reactions comprise a key step in the synthesis of large variety of molecules of biological and material interest [3] especially via cross-coupling reactions.

A variety of Co, Ni, In, Cu, and Fe, catalysts have been afterwards discoverd for the improvement of reaction conditions for S-arylation. Nevertheless, all these metal-catalyzed reactions invariably require foul-smelling, volatile, and expensive arene thiols, which are rather less available and prone to oxidative homocoupling. To have a viable alternative to thiols, use of different other sulfur sources such as thiourea, thiolates, potassium ethyl xanthogenate, thiocyanate, metal sulfides, and carbon disulfide, have been recently made to achieve the formation of diaryl thioethers. However, all the above aryl thiols sources necessitates either ligands, highly polar solvents, or long reaction time. Hence, it is important to find a practical catalytic protocol to avoid volatile and foul smelling thiols and other sulfur sources to achieve highly useful unsymmetrical aryl sulphides.




**Scheme. 1**

In this context we have made an efficient use of stable sulfonyl hydrazides as thiol proxy to bring about the practical synthesis of highly cherished unsymmetrical thioethers under MW irradiation by means of DBU acetate/CuI combination at 130 ºC in just 10 minutes (Scheme 1). The versatility, air-stability, operational simplicity, and environmental friendliness of this method highlights its potential in organic synthesis.

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**P-123**

# Multicomponent synthesis of chromenopyrimidine via Biginelli reaction and their anti-inflammatory activity

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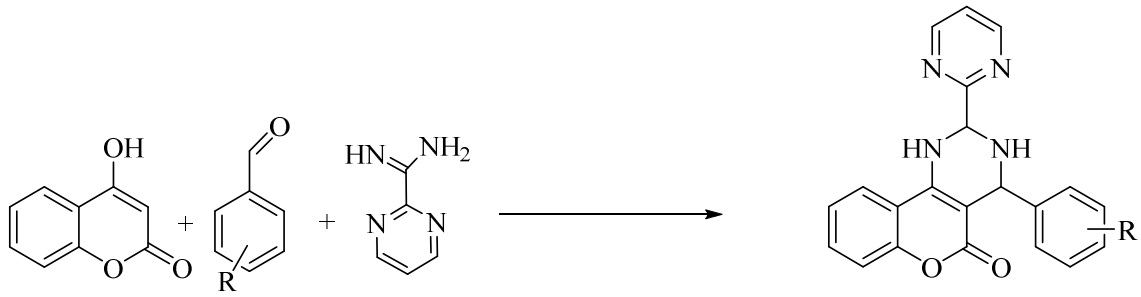
Multicomponent reactions are persuasive approach for developing a chemically diverse set of heterocyclic scaffolds with high yield. To this end, synthesis of a series of new 4-phenyl-2-(pyrimidin-2-yl)-1H-chromeno[4,3-d]pyrimidin-5(2H)-onehas been accomplished by multicomponent cyclocondensation reaction of 4-hydroxycoumarin, various substituted aldehyde, and pyrimidine-2-carboximidamide using HCl as catalyst in methanol with up to 88% yield. The anti-inflammatory studies of the title compounds are also evaluated. The detailed will be presented in poster.

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**P-124**

# Preparation and Characterization of Glutaraldehyde Cross-linked Atorvastatin Calcium Loaded Ethyl Cellulose Microsphere

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**Abstract:** The aim of the present work was to prepare glutaraldehyde cross-linkedatorvastatin calciumloadedmicrosphere in order to improve the dissolution of poorly water soluble drug and to study the effect of cross linking agent on drug release using ethyl cellulose as polymer, poly vinyl alcohol as stabilizing agentand glutaraldehyde as crosslinking agent. Microspheres were prepared by solvent evaporation method with different ratios.The prepared formulations were evaluated for interaction study by Fourier transform infrared spectroscopy andDifferential scanning calorimetry, and percentage of practical yield, drug loading, entrapment efficiency, particle size distribution analysis, surface morphology by scanning electron microscopy, *in-vitro* release study.The results showed no interaction between the drug and polymer, molecular dispersion or entrapmentof AC in the polymer matrix, percentageyield of70% to 83%, drug content of39.35% to 68.92% anddrug entrapment efficiency of 97.25% to 98.77%.Moreover the surface morphology of FIII revealed porosity on those crosslinked with glutaraldehyde.The release kinetics study revealed that the FII and FIII was predominantly controlled by first order and diffusion mechanism. From this study, it was evident that the cross-linked microsphere have tremendous potential in the area of controlled release dosage form design and also solve the problems associated with the delivery of poorly soluble drugs.

**Keywords:** Microspheres.Atorvastatin Calcium.Ethyl Cellulose.Glutaraldehyde.Solvent Evaporation Method.

P-125

## Design and evaluation of a novel pollen trap

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Pollen grains are a major source of airborne allergens and significant cause of diseases. Continuous monitoring of pollen grains released and transported in the air locally or regionally is required to determine the prevalence of various pollen types and identify intra-day and intra- annual seasonal variations over time. There are five popular pollen traps they are as follows: Burkard volumetric spore traps are widely used, because its efficiency is high but disadvantage is the efficiency varies with wind speed and particle size and also it requires electrical power and external vacuum pump. In Anderson two stage sampler the major advantage is that the volume of the air sample is known. The disadvantage of this sampler is that the efficiency varies with particle size and density and also requires uninterrupted power supply. In case of Hirst spore sampler the efficiency varies with wind speed and hence is difficult in separating the two tapes. In Durhan sampler the slides are easily loaded, inexpensive but the volume of air samplers are unknown and also catch cannot be connected to a volumetric measure of concentration. In Cour's trap, the use of wind vane does not cause any drastic changes in the composition of air borne pollen. As the above mentioned pollen traps have disadvantages, it was thought worth to design and validate a novel pollen trap to overcome these disadvantages. A modified vertical spore trap, consisting of an aluminium coated cylindrical hollow container fitted with air propeller and anemometer was designed. Air is drawn into the trap at the rate of 2 litres / ml. The airborne particles are collected on the cylindrical container. This trap was validated and the sampling efficiencies were found to be very good.

**P-126**

## Ethnomedical survey on bitter honey

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Honey is a natural product, usually sweet produced by bees using water, pollen and nectar from flowers. The biochemical composition and physical properties of natural honeys varies greatlyaccording to the plant species the bees forage. A few plants give bitter honey: *Agave* sp (Sisal), Datura sp.,Euphorbia sp.,Seneciao sp. and the like. The bitter honey are of late gaining popularity. This bitter honey is regarded as a medicine, rather than tonic or food. In the Indian system of medicine there is mention of bitter honey. Literature survey revealed that exhaustive research work has been done on honey, but little work has been done on bitter honey. FSSAI, AGMARK and Pharmacopoeial standards are available for honey, but not for bitter honey. Literature survey also revealed that bitter honey is used by the local tribal communities as a popular medicine. The ethnic claims of bitter honey has not been documented. With the advent of modernisation the ethnic knowledge of the tribals is being lost at a faster pace. Hence it was it was thought worth to carry out an ethnomedical survey on bitter honey. Preliminary survey indicated the availability of authentic bitter honey in Nilgiri District of Tamil Nadu, India. Adulteration of honey is very common. Hence it was considered that available of authentic bitter honey is an important basis for this study. The Nilgiri Biosphere reserve is the first biosphere reserve in India and is under consideration by the UNESCO for selection as a world heritage site. Among the 75 primitive tribal groups recognized by the Government of India six primitive tribes like in Nilgiri district. These six tribes are well blessed with indepth knowledge of bitter honey. A field survey was conducted among the Toda tribes at Pudu mund, Thalappatheri mund, Pagalkodu mund, Artholl mund, Kopumin mund, Thuvalkodu Mund, Taranad mund, Pillkodu mund, Garden mund, Tamilaga mund, Kunthithol mund of Nilgiri hills. During the study period, information about the traditional ethnomedical uses of bitter honey as used by Toda tribes was obtained through questionnaire survey method (Supplementary Data 1). This information was further authenticated with other members of the Toda community during the survey. The current study forms the first report to elucidate the ethno medicinal used of Bitter honey by Toda tribes to treat and control diseases in Nilgiri hills of Tamil Nadu.

P-127

# A COMPARATIVE X-RAY CRYSTALLOGRAPHIC STUDY OF METAL AND OXIDANT-FREE HIGHLY REGIOOSELECTIVE NOVEL PYRAZOLE DERIVETIVE

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**Abstract:** The novel Pyrezole derivative was synthesized by reacting 3-methyl-1-phenyl-1*H*-pyrazol-5-amine and 4-methylthiophenol in the presence of *N*-chlorosuccinimide mediated sulfenylation. A highly chemoselective $C^4$ sulfenylation of pyrazole delivered in excellent yield (95%). The target compound was characterized by spectroscopic techniques and confirmed by X-ray crystallographic studies. The crystallographic analysis suggests that the title compound crystallizes in the monoclinic space group P21/c (#14) with cell parameters a = 12.466(2) $A^{\circ}$, b = 5.9276(9) $A^{\circ}$, c = 21.389(3) $A^{\circ}$ β = 101.530(4)°, V = 1548.6(4) $A^{\circ 3}$ for Z = 4. The structure has been confirmed by direct methods and refined to $R_1$ = 0.0495 for 3,543 observed reflections and 190 variable parameters and converged.

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**P-128**

# NEGLECTED TROPICAL DISEASES (NTDs): MANIFESTATION OF THEIR OCCURRENCE AND REGIMEN TECHNIQUES TO CONQUER THE GLOBAL IMPACT

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The term "Neglected Tropical Diseases" (NTDs) characterizes a group of diseases with distinct characteristics. Some are easily treatable; others are not. The Neglected Tropical Diseases (NTDs) includes a group of chronic parasitic and related bacterial and viral infections that actually uphold poverty due to their consequences on child development, pregnancy outcome, and worker productivity. The NTDs are varying significantly in their prevalence and disease burden according to their geographic and regional occurrence. Neglected tropical diseases (NTDs) serve a major health burden in many developing countries. Pathways for research and development must be pursued in order to find new approaches and simplified strategies as well as novel diagnostics and medicines along with more comprehensive suite of tools including coordinated community-based programs, vector control, local training, education, and environmental change. In addition, comprehensive research schedule is urgently needed to develop effective diagnostic, preventive, and therapeutic arbitration to stay ahead of the evolutionary adaptation tactics of disease-causing microbes and parasites. To combat against infectious diseases will need more than purely technological solutions. It must be combination of scientific, socioeconomic, educational, environmental, and workforce strategies to overcome its global impact.

**KEYWORDS:** NEGLECTED TROPICAL DISEASES, VECTOR, PARASITE, MICROBES.

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# Antipyrine Derivatives as Anticancer Agents

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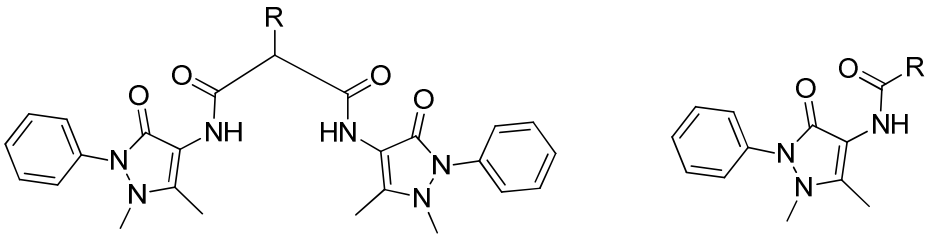
Abstract: Antipyrine has been drawn as promising structural unit in the field of medicinal chemistry. This is a heterocyclic molecule which is already reported having potent insecticidal[1], antimicrobial, anti-tumor and anti-inflamator[1] activities etc.

Cancer is a disease characterized by uncontrolled cell growth of multi-cellular organisms with seemingly unrestrained multiplication and spread within the organism of apparently abnormal forms of the organism's own cells. There is variety of cancer that is classified by the initially affected cells.

The present work deals with the synthesis and evaluation of biological activities of 4-aminoantipyrine derivatives derived from different aromatic acids. The synthesis is completed with **amide bond formation** having 92–95% yield. The structures of synthesized derivatives were established on the basis of spectroscopic and elemental analysis.




All derivatives have screened for anticancer activity on different cell lines like **colon cancer MCF-7 breast cancer, lung cancer** etc. The screening results have shown that compounds most of them having moderate to good anti-cancer activity. Some of them are in process of biological evaluation for $IC_{50}$ value on different cell lines.

The bioactivity of these derivatives has also been evaluated with respect to Lipinski's rule of five using mol-inspiration and chem-informatics softwares.

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