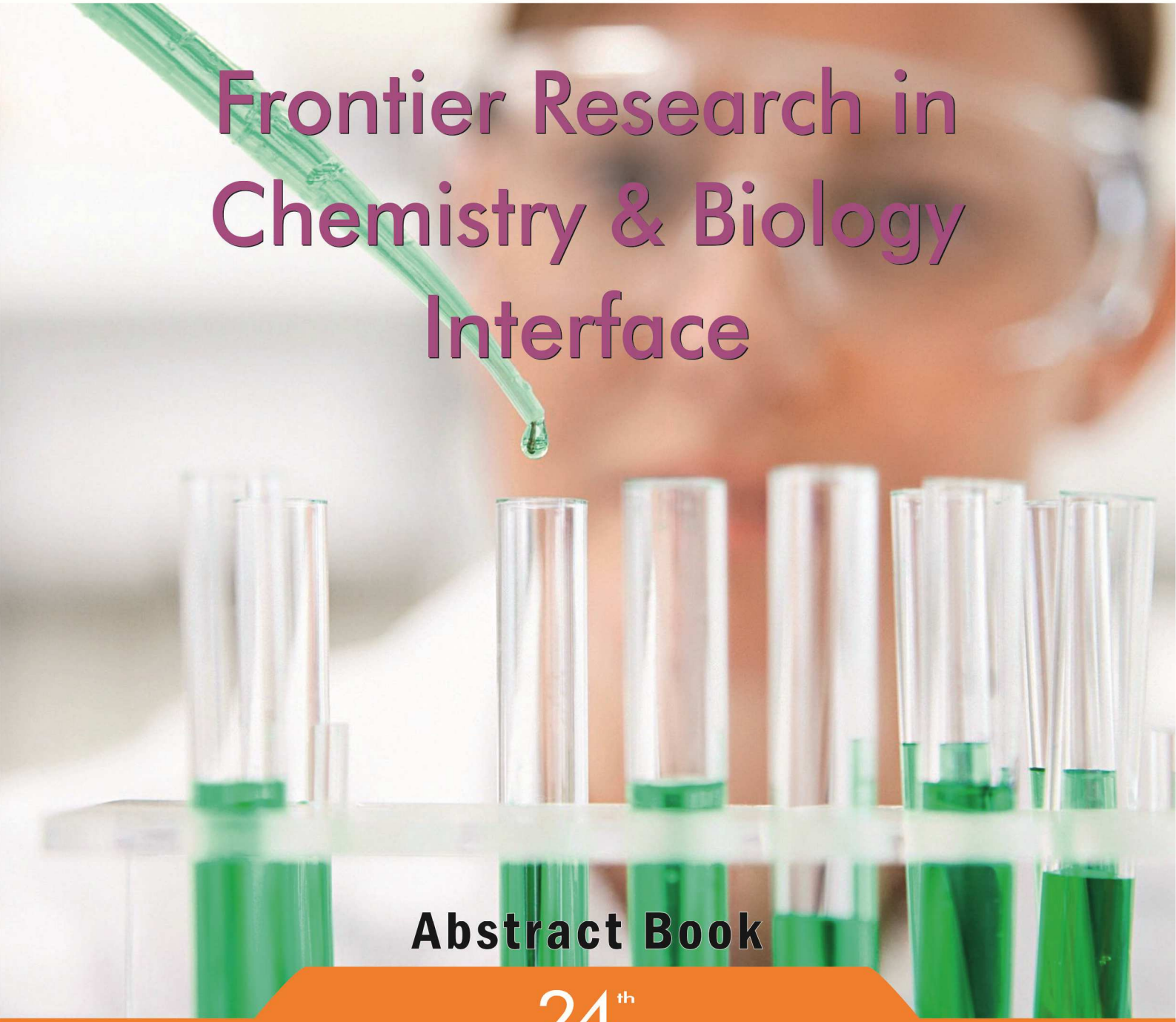
MANIPAL UNIVERSITY
JAIPUR

Frontier Research in Chemistry & Biology Interface



Abstract Book

24th ISCB INTERNATIONAL CONFERENCE (ISCBC-2018)

11-13 January 2018
at
Manipal University Jaipur
Rajasthan, India

Jointly Organized by:
Indian Society of Chemists & Biologists
Manipal University Jaipur

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ISCBC-2018

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Manipal University Jaipur

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Smt. Vasundhara Raje
Chief Minister, Rajasthan

सत्यमेव जयते

VASUNDHARA RAJE
CHIEF MINISTER RAJASTHAN

Message

I am happy to learn that the **Department of Chemistry, Manipal University, Jaipur** is organizing the 24th ISCB International Conference in association with Indian Society of Chemists and Biologists on **Frontier Research in Chemistry & Biology Interface** on 11-13 January, 2018.

I hope that this conference would provide a platform for the participant researchers, scientists and students to share knowledge about innovations and advances in research in the drugs and pharmaceutical sector.

I wish the event the very best.

Vasundhara Raje.

(Vasundhara Raje)

Smt. Kiran Maheshwari
Minister, Rajasthan

किरण माहेश्वरी
मंत्री
उच्च, तकनीकी एवं संस्कृत शिक्षा,
विज्ञान एवं प्रौद्योगिकी विभाग
राजस्थान सरकार

Kiran Maheshwari
Minister
Higher, Technical and Sanskrit Education,
Science and Technology Department
Government of Rajasthan

सत्यमेव जयते

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Jaipur, Date 30.12.17

MESSAGE

I am happy to note that Manipal University Jaipur is organizing the 24th ISCBC conference from January 11-13, 2018.

The theme of the conference, "Frontier Research in Chemical & Biological Interface" speaks volumes of the interdisciplinary research, which is the need of the hour. The theme is not only interesting but relevant to the present scenario where there is an urgent need for researchers and academicians to join hands and discuss innovative ideas and strategies to find answers to fundamental questions such as drug designing, and address practical challenges in the pharmaceutical industry, biotechnology, agricultural biotechnology, environmental science, and medicine.

I am sure that renowned scientists from all around the globe, people from industries and academia who are part of this conference, will be able to articulate their insight and suggest suitable technologies for the benefit of the society as a whole.

Kiran Maheshwari
(Kiran Maheshwari)

Prof. Anamik Shah
Vice Chancellor, Gujarat Vidhyapeeth
President, ISCB

Dr. P.M.S. Chauhan
Chief Scientist and Professor,
CDRI, Lucknow
General Secretary, ISCB

Message

We are very happy to inform you that the Indian Society of Chemists and biologists, Lucknow, jointly organising its 24th international conference with Manipal University, at Jaipur, India from 11th – 13th January, 2018 (Thu-Sat).

It is a matter of great pleasure that the focal theme of the 24th International Conference of ISCB on 'Frontier Research in Chemistry & Biology Interface. During above conference researcher are going to discuss self reliance, sustainability & affordability of pharmaceutical substances by improving process chemistry through innovation so that India can be more competitive and self reliant on Pharma products, drug intermediates & finished formulations. Scientists across the globe, especially from USA, Greece UK, France, Poland, Slovenia, Belgium, Sweden, Italy and many other countries will participate as keynote/invited speakers to address above mentioned issues. The entire conference will be addressed by more than 60 senior scientists & professors as key-note/invited speaker while it will attract more than 600 young researchers & post doctoral researchers from entire country who will take part as oral/poster presentations.

We are glad that the scientific committee is bringing out an abstracts book covering the presentations to be made during ISCBC-2018. Our sincere thanks are due to the members of organizing committee. During this conference a number of eminent scientists and technologists of the country and overseas will be discussing the trends, prospects and future directions of research. We look forward to fruitful deliberations in extremely interesting areas of scientific research. We are happy that an extensive and comprehensive scientific program is arranged. The scientific program beside inaugural function includes 1 Keynote lecture, 12 plenary lectures, 48 invited lectures by the eminent scientists from India and abroad. 64 Oral presentations by the young researchers are scheduled. The most heartening feature of the conference is that it is being participated with a number of young scientists and Ph. D. students and presentations are schedules in three poster sessions. On behalf of ISCB we are looking for the galaxy of speakers and young participants who made this conference a memorable event. We extend our warm welcome to all National and International delegates from pharmaceutical companies, research organization, universities and academic institutes wish them very happy stay at Jaipur. Now Finally I take this opportunity to express my sincere thanks and gratitude to members and office bearers of organizing committee of 24th International Conference (ISCBC-2018).

Anamik Shah

(Prof. Anamik Shah)
President, ISCB

PMSchauhan

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

MANIPAL UNIVERSITY
JAIPUR

Dr. K. Ramnarayan
Chairperson
Manipal University Jaipur

Message from Chairperson

I am delighted that the 24th ISCBC conference on *Frontier Research in Chemistry & Biology Interface* is being organized by Department of Chemistry from January 11-13, 2018 in association with the Indian Society of Chemists and Biologists.

The 24th ISCBC conference covers wide range of research areas in the interface of chemistry and biology. I earnestly hope that the participants, delegates especially the young researchers will derive maximum benefit from the deliberations on important topics related to challenges involved in the dynamic and fast moving field of drug research.

I extend a warm welcome to the eminent scientists, academicians not only from India but across the world and also representatives from industries participating in this conference.

I applaud the Department of Chemistry for this initiative and wish that this conference is a rewarding experience for everyone involved.

Best wishes.

Dr. K Ramnarayan
Chairperson, MUJ

Manipal University Jaipur, Dehmi Kalan, Near GVK Toll Plaza Jaipur-Ajmer Expressway, Jaipur, Rajasthan 303 007
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MANIPAL UNIVERSITY
JAIPUR

Prof. Sandeep Sancheti
PhD (UK), FIETE, FIE (I), MIEEE
President

Message from President, Manipal University Jaipur

I am delighted to learn that Department of Chemistry is organizing the 24th ISCBC conference from January 11-13, 2018 in association with Indian Society of Chemists and Biologists. It is a welcome initiative that would bring together domain experts, researchers and students from a number of institutions including those from abroad to exchange ideas, share their research findings and build new collaborations in the field of its theme areas - *Frontier Research in Chemistry & Biology Interface.* Let me congratulate the organizing committees for their initiative and efforts to shape such a meaningful programme.

I believe that the conference will not only provide a forum for the participants to exchange scientific views and debate on aforementioned issues, but will also lead to generation of new ideas and interests. It is clear that research in Chemistry & Biology would impact the society and industry in the form of health services and a variety of other domains. To this end Manipal University Jaipur is regularly collaborating with research organizations and industries to create a stimulating environment for research and development in all important fields of its activities and in particular that of Chemistry and Bio-sciences.

On behalf of Manipal University Jaipur I would like to extend our warm welcome to all participants and wish a huge success to ISCBC conference in its endeavour of promoting research.

(Prof Sandeep Sancheti)

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MANIPAL UNIVERSITY
JAIPUR

Message from Chairman, ISCBC-2018

I am pleased to share that Department of Chemistry, Manipal University Jaipur is organizing 24th ISCB conference on the theme of *Frontier Research in Chemistry & Biology Interface* from January 11-13, 2018 in association with Indian Society of Chemists and Biologists. The conference shall have an august congregation of around 500 leading researchers, industry experts, pharmacologists and academicians and other allied professionals from India and abroad. The deliberations in the 3 day conference shall focus on the different domains of research in the areas of both chemistry and biology and their interface. I am sure that the gainful discussions and presentation of papers on the latest research in drug discovery and therapeutics will be the hallmark of the conference and it will provide an opportunity for our faculty and students to interact personally with them to understand the importance of various domains of drug research.

I would like to extend a warm welcome to all the participants and request all the stakeholders to participate meaningfully to make the conference a success.

Suhag

Prof Vandana Suhag

Manipal University Jaipur, Dehmi Kalan, Near GVK Toll Plaza Jaipur-Ajmer Expressway, Jaipur, Rajasthan 303 007
dir. 91 14 1399 9100 *fax.* 91 14 1399 9102 www.jaipur.manipal.edu

Prof G C Tikkiwal
Dean, Faculty of Science
Manipal University Jaipur

Message

It gives me immense pleasure to learn about that 24th ISCB conference on "*Frontier Research in Chemistry & Biology Interface*", organized by the Department of Chemistry at Manipal University Jaipur in association with Indian Society of Chemists and Biologists from January 11-13, 2018.

The conference covers wide spectrum of areas such as drug design, natural products, synthetic chemistry, bio-nanotechnology and agricultural biotechnology research, pharmaceutics, pharmacokinetics, toxicology and clinical research, which are the different domains of research in the areas of both chemistry and biology and their interface.

I am happy to learn that around 500 participants which includes renowned academicians and researchers from India and abroad will be participating in the conference.I believe that the brain storming sessions on the interface of both Chemistry and Biology will helpscience in a big way, fostering the growth of basic research in both the areas for the benefit of the society.

I wish the event and its organizers all success.

Prof G C Tikkiwal
Dean, Faculty of Science
Manipal University Jaipur

Prof. Babita Malik
Convener
ISCBC-2018

Dr. Nitu Bhatnagar
Organizing Secretary
ISCBC-2018

Dr. Tanmoy Chakraborty
Organizing Secretary
ISCBC-2018

Welcome Message from Organizing Team

It is our great pleasure to welcome a galaxy of scientists, academicians and delegates to this 3 day International Conference on **'Frontier Research In Chemistry & Biology Interface'** organized by **Department of Chemistry**, Manipal University Jaipur **from January 11-13, 2018** in collaboration with **Indian Society of Chemists and Biologists.**

24th ISCBC conference is a multidisciplinary conference includes themes related to chemistry and biology interface. The vision of the ISCBC conference is to provide a forum for in-depth assessment of the challenges involved in the dynamic and fast moving field of Drug research ISCB conference has prime objective to provide an opportunity for a close interaction of scientists with varied interests in diverse fields of the research. It provides a common platform and opportunities to the researchers in the areas of chemical and biological sciences and other related areas to interact with each other. It will bring together leading chemists, medicinal chemists, pharmacologists, and other allied professionals to discuss and present the latest developments in drug discovery and therapeutics.

Eminent scientists from India and abroad will present their work in the conference. The conference will have total nine lecture sessions and three poster sessions. These lecture sessions will comprise of 1 Keynote lecture, 12 plenary lectures, 48 invited lectures by the eminent scientists from India and abroad. 64 Oral presentations by the young researchers are also scheduled. Apart from this, more than 300 young researchers will present their work through posters. Distinguished scientists like **Prof. M. M. Sharma, Dr. Girish Sahni, Director General, CSIR and Secretary, DSIR** will address in the conference.

A team comprising of students and faculty members have been working day night to give shape to this international conference. On behalf of organizing committee, we take this opportunity to congratulate the entire team, especially students, faculty members and staff for their dedication and sincere efforts to make this international conference a memorable one.
We take this opportunity to thank all the authors who have contributed excellent papers and our sponsors and exhibitors for their strong support. Thanks are also due, to the members of the National and International Advisory Committee and many volunteers whose generous help and support have made this conference possible.

On behalf of the organizing committee and our own behalf we feel privileged to extend our heartiest and warm welcome to all the esteemed guests and delegates.

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24th ISCB International Conference (ISCBC-2018)

Frontier Research in Chemistry & Biology Interface

January 11-13, 2018

Jointly Organized by
Indian Society of Chemists & Biologists, Lucknow, India
Manipal University Jaipur, Jaipur, India
at
Manipal University Jaipur, Jaipur, India

SCIENTIFIC PROGRAMME

Thursday, January 11, 2018

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	**Prof. Vandana Suhag, Registrar, MUJ & Chairman, ISCBC-2018**
10.45 AM	About Manipal Group	**Prof. K. Ramnarayan, Chairperson, MUJ**
10:50AM	Introduction to ISCB	**Dr. P.M.S. Chauhan, Gen. Secretary ISCB**
11:00AM	Presidential Address	**Prof. Anamik Shah, President ISCB**
11:10AM	About Manipal University Jaipur	**Prof. Sandeep Sancheti, President, MUJ**
11:15AM	ISCB Award Distribution	
11:30AM	Address by Chief Guest	**Dr. Girish Sahni, Secretary, DSIR and DGCSIR**
11:40AM	Address by Guest of Honour	**Prof. M.M. Sharma, Institute of Chemical Technology, Mumbai** **Pangs of process development and linkages of chemistry with biology & material science**
11:45AM	Keynote Lecture	
12:15 PM	Vote of Thanks	**Prof. Babita Malik, Convenor, ISCBC-2018**
12.20 PM - 12.30 PM	**High Tea**	

Session – I

Chairperson: Prof. Fraser Fleming,

PL-1 12.30 PM - 1.00 PM	**Girolamo Cirrincione** Professor of Medicinal Chemistry, University of Palermo, Pro Rector for Research, Palermo, Italy **Marine Alkaloid Analogs Inhibit Kinases and Growth of Cancer Stem Cells**
1.00 PM - 2.00 PM	**Lunch**
ISCB Award Lectures 2.00 PM - 2.25 PM	**Janez Plavec (ISCB Pof. Jyoti Chatterji Prize for Excellence-2018)** Head of Slovenian NMR center, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia **NMR studies of G-rich DNA fragments that fold into G- and AGCGA-quadruplexes**
2.25 PM - 2.50 PM	**A. K. Ganguly (ISCB Excellence Award 2018)** Director, INST, Mohali, India **Abstract Awaited**
2.50 PM - 3.05 PM	**Rajneesh Mishra (ISCB Young Scientist Award 2018)** Associate Professor, Indore, India **Abstract Awaited**
3.05 PM - 3.20 PM	**Vijay Kumar Prajapati (ISCB Young Scientist Award 2018)** Assistant Professor, Department of Biochemistry, School of Life Sciences, Central University of Rajasthan, Ajmer, India **Abstract Awaited**
3.20 PM - 3.35 PM	**Vinita Chaturvedi (ISCB Distinguish Women Scientist Award 2018)** Senior Principal Scientist, Biochemistry Division, Central Drug Research Institute, Lucknow, India **Abstract Awaited**
3.35 PM - 3.50 PM	**Mahesh C. Sharma (ISCB Best Teacher Award 2018)** Associate Professor, Convener, Board of Studies in Chemistry, Natural Products Laboratory, Centre for Advanced Studies Department of Chemistry, University of Rajasthan, Jaipur, Rajasthan, India **Abstract Awaited**
3.50 PM - 4.05 PM	**Dharmendra Singh (ISCB Best Thesis Award 2018)** IIT Madras, Chennai, India **Abstract Awaited**
4.05 PM - 4.30 PM	**Tea**

Parallel Session – II A

Chairpersons: Prof. Jyoti Chattopadhyaya, Prof. A.K. Sinha

PL-2 4.30 PM - 5.00 PM	**Barbara Zajc** Department of Chemistry and Biochemistry, The City College of New York, New York, USA

	Synthesis of Regiospecifically Fluorinated Polycyclic Aromatic Hydrocarbons and Influence of Fluorine Atom
PL-3 5.00 PM -5.30 PM	**S. Chandrasekhar** Director, CSIR-Indian Institute of Chemical Technology, Hyderabad, India **Abstract Awaited**
PL-4 5.30 PM - 6.00 PM	**Anil Kumar Singh** IIT Mumbai, Former Vice Chancellor, University of Allahabad, India **Understanding Retinal-Bound Photoreceptors through Bioorganic Chemistry**
IL-1 6.00 PM - 6.20 PM	**Mukund S. Chorghade** President and Chief Scientific Officer, THINQ Pharma / THINQ Discovery, and Chorghade Enterprises, USA **Chemosynthetic Livers: Predict, Prepare and Prove the Structure, Activity and Toxicity of Drug Metabolites**
IL-2 6.20 PM - 6.40 PM	**Arun K. Sinha** Chief Scientist and Professor (AcSIR), Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Natural and Unnatural Phenolic Based Small Molecules: Green Chemical Synthesis and their Biological Evaluation**

Parallel Session – II B

Chairpersons: Prof. Anil Kumar Singh, Dr. S. J. S. Flora

PL-5 4.30 PM - 5.00 PM	**Fraser Fleming** Professor and Department Head, Drexel University, USA **Strategic Alkylations of Nitriles and "Isonitriles"**
PL-6 5.00 PM - 5.30 PM	**Mahesh K. Lakshman** Department of Chemistry and Biochemistry, The City College of New York, New York, USA **(Diacetoxyiodo)benzene-Mediated Cyclization Reactions of N^6-Aryl and N^6-([1,1'-Biaryl]-2-yl) Adenosine Derivatives**
IL-3 5.30 PM -5.50 PM	**Virinder S Parmar** Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi, India **Development of Novel Polymeric Nanomaterials, Nanocomposites and Dendrons *via* Biocatalytic Routes**
IL-4 5.50 PM - 6.10 PM	**Ashok K Prasad** Professor, Department of Chemistry, University of Delhi, Delhi, India **Sugar Modification and Its Value Added Application**
IL-5 6.10 PM - 6.30 PM	**Dipankar Koley** Scientist, CSIR-Central Drug Research institute, Lucknow **Asymmetric Synthesis of Izidine Alkaloids: Connection between Acetal and Hydroxylactam**

Poster Session –I

Chairpersons: Prof. Desh Deepak, Dr. Jawahar Lal, Dr. Jaybir Sngh, Dr. Rahul Shrivastava

6.30 PM – 7.30 PM	**Poster Number 1 to 130**
7.30 PM – 8.30 PM	**Cultural Programme**
8.30 PM	**Dinner**

Friday, January 12, 2018

Poster Session – II

Chairpersons: Prof. Athina Geronikaki, Dr. Rakesh Shukla, Dr. Jaybir Singh

8.30 AM – 9.30 AM	**Poster Number 131 to 260**

Parallel Session – III A

Chairpersons: Prof. Anamik Shah, Prof. A. K. Goswami

PL-7 9.30 AM - 10.00 AM	**Samir Zard** Professor and former Editor Tetrahedron Letters, Directeur de Recherche CNRS (DRCE) et Professeur à l'École Polytechnique, France **Reversible Reservoirs for Radicals. A Powerful Strategy for the Creation of Carbon-Carbon Bonds**
IL-6 10.00 AM - 10.20 AM	**Sun CHOI** College of Pharmacy & Graduate School of Pharmaceutical Sciences, Ewha Womans University, Seoul, Korea **Exploration of protein motion, allostery, andintramolecular signaling of GPCR, and its implication in drug design**
IL-7 10.20 AM - 10.40 AM	**S. J. S. Flora** Director, National Institute of Pharmaceutical Education and Research (NIPER), ITI Compound, Raebareli 229010, India **Monoisoamyl DMSA, a ray of hope for the treatment of Chronic Arsenicosis-Journey from lab to human trial**
IL -8 10.40 AM - 11.00 AM	**Ashoke Sharon** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Neplanocin Derived Analogs: A potential scaffold as anti-HBV agents**
IL -9 11.00 AM - 11.20 AM	**Bapu B. Shingate (ISCB Best Teacher Award 2018)** Assistant Professor, Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, India **Ionic hydrogenation-directed stereoselective construction of C-20(H) stereogenic center in steroid side chains: Scope and limitations**
IL -10 11.20 AM -11.40 AM	**Farukh Arjmand** Department Of Chemistry, Aligarh Muslim University, Aligarh, India **Insights to the mechanistic pathway of tailored de novo antitumor**

	Cu(II)/Zn(II) drug candidates: Structure elucidation and biological studies for validation of target sites
11.40 AM - 11.50 PM	**Tea**

Parallel Session – III B

Chairpersons: Dr. PMS Chauhan, Prof. Victor Kartsev

PL-8 9.30 AM - 10.00 AM	**Jyoti Chattopadhyaya** Professor & Chair, Program of Chemical Biology, Dept. of Cell & Molecular Biology, Uppsala University, Sweden **How RNase HI (E. coli) promoted site-selective hydrolysis works on RNA in duplex with carba-LNA and LNA substituted antisense strands in the antisense strategy?**
IL-11 10.00 AM -10.20 AM	**Sergii Rudiuk** Permanent Researcher, Department of Chemistry, Ecole Normale Supérieure, 75005 Paris, France **NON-COVALENT APPROACHES FOR THE DYNAMIC CONTROL OF DNA AND DNA-BASED MATERIALS**
IL-12 10.20 AM - 10.40 AM	**Gopi Mohan C.** Asso. Professor, Nanosciences, Center for Nanosciences, Kochi, India **Abstract Awaited**
IL -13 10.40 AM - 11.00 AM	**Satpal Singh Badsara** Assistant Professor, Centre of Advanced Study, Department of Chemistry, University of Rajasthan, Jaipur, India **Metal Free Syntheses of Thioethers: Reactivity, Scope and Challenges**
IL -14 11.00 AM - 11.20 AM	**Amit Mishra** Assistant Professor, Department of Biology, Indian Institute of Technology Jodhpur, Jodhpur, India **How ProteostasisDefects Contribute In Ageing And Neurodegeneration?**
IL -15 11.20 AM -11.40 AM	**Jawahar Lal** Senior Principal Scientist & Head, Pharmacokinetics & Metabolism Division, CSIR-Central Drug Research Institute, Lucknow, India **Assessment of Bioenhancing potential of Lysergol**
11.40 AM - 11.50 PM	**Tea**

Parallel Session - IV A

Chairpersons: Dr. Rakesh Shukla, Prof. Rajesh Dhakarey

PL-9 11.50 AM - 12.20 PM	**Victor Kartsev** Full member of RANS, Honorary Academician of Russian Academy of Arts, VP, CSO&CEO InterBioScreen, Russia **THIAZOLE AND THIAZOLIDINONE DERIVATIVES OF NATURAL ORIGIN AS ANTIMICROBIAL AGENTS**

IL-16 12.20 PM - 12.40 PM	**Ramesh Babu Boga** BogaR Laboratories LLC, PO Box 1554, Suwanee, GA 30024, USA **Chemical Diversity of Benzimidazoles: Design, Synthesis, and Biological Applications**
IL-17 12.40 PM - 1.00 PM	**Rachna Sadana** Assistant Professor of Biology and Biochemistry, Department of Natural Sciences, University of Houston-Downtown, One Main Street, Houston, TX-77002 **The future of the PhD: A Careers Away from the Bench?**
IL-18 1.00 PM - 1.20 PM	**Namrata Rastogi** Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow 226031, India **SILYL DIAZOENOLATES AS NUCLEOPHILES IN VISIBLE LIGHT PHOTOREDOX CATALYZED MANNICH REACTION**
IL-19 1.20 PM - 1.40 PM	**Yasmeen Pervez** Professor, Dept. of Chemistry, CSIT, Durg, India **Carbonaceous fractions in Indoor Air Due to Burning Activities: Threat to Health and Climate**
1.40 PM - 2.20 PM	**Lunch**

Parallel Session - IV B

Chairpersons: Dr. Manjunath Ghate, Dr. Rakhi Bakshi

IL-20 11.50 AM - 12.10 PM	**Dalip Kumar (ISCB Best Teacher Award 2018)** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **Nature-inspired Chemical Design and Efficient Syntheses of Drug-like Nitrogen Heterocycles**
IL-21 12.10 PM - 12.30 PM	**Devesh M Sawant** Asst. Professor, Department of Chemistry, School of Chemical Sciences and Pharmacy, Central University of Rajasthan (CURAJ), Bandarsindri, Rajasthan-305817, India **Transition-metal catalyzed novel and sustainable strategies for the synthesis of bioactive heterocycles**
IL-22 12.30 PM - 12.50 PM	**R. K. Singh** Division of Toxicology & Experimental Medicine, CSIR-central Drug Research Institute, Lucknow-226031, India **Invention of A New Molecule RISUGadv in India for the Prevention of Prostate Cancer**
IL-23 12.50 PM - 1.10 PM	**Brijesh Kumar** Senior Principal Scientist, Sophisticated Analytical Instrument Facility (SAIF), CSIR-Central Drug Research Institute, Lucknow, India **LC-MS/MS methods to identify characterize and determine bio active phytochemicals and study their variation in *Indian Medicinal* Plants**
IL-24	**Ram Prakash** Senior Scientist, CEERI Pilani, India

1.10 PM - 1.30 PM	**Plasma for Chemistry and Biology Interface**
1.30 PM - 2.20 PM	**Lunch**

Parallel Session - V A

Chairpersons: Prof. G.C.Saxena, Dr. K. Deo

PL-10 2.20 PM - 2.50 PM	**Kevin H. Shaughnessy** Professor and Chair, Department of Chemistry, The University of Alabama, Tuscaloosa, AL, USA **FROM MECHANISTIC UNDERSTANDING TO CATALYST APPLICATION: DEVELOPING NEW CATALYSTS FOR BOND-FORMING REACTIONS**
IL-25 2.50 PM - 3.10 PM	**Manoj Kumar** Project Director, DRDL, Hyderabad, India **Abstract Awaited**
IL-26 3.10 PM - 3.30 PM	**Prashanth N Suravajhala** Department of Biotechnology and Bioinformatics, Birla Institute of Scientific Research, Statue Circle, Jaipur 302001, RJ, India **Myths of Identifying Long Non-coding RNAs using Whole Exome Sequencing: Challenges and Perspectives**
O-1 3.30 PM - 3.40 PM	**Poonam** Department of Chemistry, Miranda house, University of Delhi, India **DESIGN AND SYNTHESIS OF FUNCTIONALIZED ORGANIC-INORGANIC HYBRID NANOMATERIALS AND ITS APPLICATION IN ENVIRONMENTALLY BENIGN REACTIONS**
O-2 3.40 PM - 3.50PM	**Shovan Mondal** Assistant Professor, Department of Chemistry, Syamsundar College, Shyamsundar, Burdwan,West Bengal, India **"Sultam" and "Sultone" chemistry in Modern Research**
O-3 3.50 PM - 4.00 PM	**Neetu Bansal** Department of Chemical Engineering, University of Pretoria, Pretoria 0002 **Chromium in Environment, Its Toxic Effect from Chromite Mining and Ferrochrome Industry: South Africa**
4.00 PM - 4.20 PM	**Tea**

Parallel Session - V B

Chairpersons: Prof. G.C. Tikkiwal, Dr. Jyoti Joshi

IL-27 2.20 PM - 2.40 PM	**Anil Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **Synthesis of Polyheterocyclic Compounds *via* Transition Metal Catalyzed C-H Functionalization**
IL-28	**Sachin Shymasundar Laddha**

2.40 PM - 3.00 PM	Principal, PremlilaVithaldas Polytechnic, SNDT Women's University, Mumbai, India **Phosphodiesterase Enzyme: Promising target for Medicinal Chemist**
IL-29 3.00 PM - 3.20 PM	**Ravi P. Singh** Department of Chemistry, Indian Institute of Technology-Delhi, HauzKhas, New Delhi, India **Transition Metal Catalyzed Dehydrogenative Cross-Coupling: Direct Access to polycyclic Heteroarenes**
O-4 3.20 PM - 3.30 PM	**Zohra Benfodda** University of Nîmes, EA7352 CHROME, Rue du Dr G. Salan, 30021 Nîmes cedex 1, France **Rational design, synthesis and antimicrobial properties of thiophene derivatives that inhibit bacterial histidine kinases**
O-5 3.30 PM -3.40 PM	**Brijesh Rathi** Department of Chemistry, Massachusetts Institute of Technology, Massachusetts Avenue, Cambridge MA 02139 USA **MULTISTAGE INHIBITORS OF MALARIA PARASITE VITAL FOR MALARIA ERADICATION**
O-6 3.40 PM -3.50 PM	**Charan Kumar Ramineni** Doctorate student, Biochemistry, University of Massachusetts Lowell, MA, USA **Developability Assessment of an IgG2 Monoclonal Antibody Prior to Commencement of Process Development**
4.00 PM - 4.20 PM	**Tea**

Parallel Session - VI A

Chairpersons: Prof. Babita Malik, Dr. Neelima Gupta

IL-30 4.20 PM - 4.40 PM	**Ashu Chaudhary** Department of Chemistry, Kurukshetra University, Kurukshetra, India **"GREENER" CHEMICAL SYNTHESES FOR BIOINSPIRED METALLO MACROCYCLES: A WINDOW INTO MEDICINAL CHEMISTRY**
IL-31 4.40 PM - 5.00 PM	**Sandeep Verma** Prof. & Head, Dept. of Chemistry, IIT Kanpur, India **Neuronal Gasotransmitter Delivery with a Redox Trigger**
IL-32 5.00 PM - 5.20 PM	**RakshVirJasra** Senior Vice President (R&D), Reliance Industries Limited, India **Catalysis for Green Chemical Production**
IL-33 5.20 PM - 5.40 PM	**Ajay K. Sah** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, India **Cu(II) Complexes of D-glucose derivatives and their application in oxidation reactions**
IL-34	**S. Venkata Mohan**

5.40 PM - 6.00 PM	Bioengineering and Environmental Sciences Lab, EEFF Department, CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad, India **Waste Biorefinery for Chemical and Fuels**
IL-35 6.00 PM - 6.20 PM	**Sangeeta Jha** Department of Chemistry, Sikkim Manipal Institute of Technology, Majitar, East Sikkim, India **HIGH PERFORMANCE POLYMERIC NANO COMPOSITE AND ITS TECHNOLOGICAL APPLICATIONS**

Parallel Session - VI B

Chairpersons: Dr. A. K. Dwivedi, Dr. S.K. Singh

IL-36 4.20 PM - 4.50 PM	**Anshu Dandia** Retd. Prof. Dept. of Chemistry, Rajasthan University, India **Waste Biorefinery for Chemical and Fuels**
IL-37 4.50 PM - 5.10PM	**Devdutt Chaturvedi** Department of Chemistry, School of Physical & Material Sciences, Mahatma Gandhi Central University, Motihari-845401(East Champaran), Bihar, India. **Chemistry of carbon dioxide: Greener applications & synthetic explorations**
IL-38 5.10 PM - 5.30 PM	**Shamima Hussain** Scientist-E, UGC-DAE CSR, Kalpakkam Node, Kokilamedu-603104, India **Correlating Morphology and bonding environment in freestanding thin films**
IL-39 5.30 PM - 5.50 PM	**Shamsh Pervez** Professor, Dept. of Chemistry, PRSS University, Raipur, India **Air Quality Studies to Address Uncharted Sources of urban climate in India**
IL-40 5.50 PM - 6.10 PM	**I.K. Sharma** Prof. Dept. of Chemistry, Rajasthan University, India **Abstract Awaited**

Poster Session – III

Chairpersons: Dr. Dipankar Koley, Dr. Namrata Rastogi

6.20 PM – 7.30 PM	**Poster Number 261 onwards**
7.30 PM – 8.30 PM	**Cultural Programme**
8.30 PM	**Dinner**

Saturday, January 13, 2018

Parallel Session – VII A

Chairpersons: Prof. Vandana Suhag, Dr. K.S. Lakshmi

PL-11	**Athina Geronikaki** Department of Pharmaceutical Chemistry, Aristotle University, Greece

8.30 AM - 9.00 AM	**NOVEL THIAZOLIDIN-4-ONE DERIVATIVES WITH POTENT HIV-1 REVERSE TRANSCRIPTASE INHIBITORY ACTIVITY. DIVERGENCE FROM NON-COMPETITIVE INHIBITION MECHANISM**
IL-41 9.00 AM -9.20 AM	**K. Shankar Rao** Professor & Head, Dept. of Rasashastra, National Institute of Ayurveda, Jaipur, India **USE OF METALS & MINERALS AS MEDICINE AND CONCEPT OF SHODHANA & MARANA : A NEW PHARMA CONCEPT**
IL-42 9.20 AM - 9.40 AM	**Arunava Agarwala** Depatment of Chemistry, Manipal University Jaipur, Jaipur, India **Surface modification of metal oxides by dopant containing organic compounds and application in surface doping of silicon nano-structure**
O-7 9.40 AM - 9.50 AM	**Davood Askari** Master,SGPC, Mashhad, Iran **Reduce energy consumption and greenhouse gases emitting in the distillation unit using the feed- product heat exchanger**
O-8 9.50 AM - 10.00 AM	**Jyoti Singh** Institute of Pharmacy, RITM-AKTU, Lucknow **COMPUTER AIDED DRUG REPOSITIONING AND BIOLOGICAL EVALUATION AGAINST PARKINSON DISEASE**
O-9 10.00 AM - 10.10 AM	**Raj Kumar** Laboratory for Drug Design and Synthesis, Centre for Pharmaceutical Sciences and Natural Products, Central University of Punjab, 151 001, Bathinda, India **Design, Synthesis and anticancer activity of Imidazo[1,2-a]quinoxaline as Inhibitors of Tubulin Polymerization**
O-10 10.10 AM - 10.20 AM	**Jaybir Singh** Department of Pharmacy, Dr. B. R. Ambedkar University, Agra (U.P.) India **Design and Evaluation of Orodispersible Tablets Using Combination of Superdisintegrants**
O-11 10.20 AM -10.30 AM	**Anant Kapdi** Institute of Chemical Technology, Mumbai, Nathalal road, Matunga, Mumbai-400019, India **Sustainable Palladium Catalysis for the Synthesis of Multi-functional Nucleosides in Water**
O-12 10.30 AM -10.40 AM	**Purnima Nag** School of Basic Sciences, Jaipur National University, Jaipur, India **BIOSYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL ATIVITY OF SILVER NANOPARTICLES USING LEAF EXTRACT OF THUJA ORIENTALIS**
O-13 10.40 AM -10.50 AM	**Ganesan Krishnamoorthy** Chemical Sciences & Technology Division, CSIR-North East Institute of Science & Technology, Jorhat - 785 006, Assam, India **DEVELOPMENT OF IONICALLY CROSS LINKED PHOTORESPONSIVE (TPCC4) CHITOSAN NANOPARTICLE FOR DRUG DELIVERY**
O-14	**K. Gajanan** Associate Professor, Dept. of Applied Chemistry ,KITS Ramtek-441 106 ,Nagpur,

10.50 AM -11.00 AM	M.S., India **Fate of Organochloro and other Pesticide Residues in Soil and Aquatic Environment and their Neuro-toxic Effects**
O-15 11.00 AM -11.10 AM	**Ali Mohd Lone** Laboratory of Organic Synthesis, Govt. Degree College for Women Baramulla-193101, India **A general, flexible, ring closing metathesis (RCM) based strategy for accessing the fused furo[3,2-b]furanone moiety present in diverse bioactive natural products**
O-16 11.10 AM -11.20 AM	**Reetam Kaushik** Department of Chemistry, University of Delhi, Delhi, India **Synthesis and characterization of Lanthanide substituted transition metal containing inorganic-organic hybrid polyoxometalates**
O-17 11.20 AM -11.30 AM	**Samir Y. Abbas** Organometallic and Organometalloid Chemistry Department, National Research Centre, Cairo, Egypt **Utilizing of *N*-(4)-(benzo[d][1,3]dioxol-5-yl) thiosemicarbazide in the syntheses of various novel types of thiosemicarbazone derivatives: synthesis and antiviral evaluation**
11.30 AM - 11.40 PM	**Tea**

Parallel Session – VII B

Chairpersons: Prof. Mahesh Sharma, Prof. N.C. Desai

PL-12 8.30 AM - 9.00 AM	**Karol Grela** Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Poland **Olefin metathesis with modern ruthenium catalysts: applications in basic research and in industrial production**
IL-43 9.00 AM -9.20 AM	**ACS International India Pvt. Ltd.** ACS International India Pvt. Ltd, India **Abstract Awaited**
IL-44 9.20 AM - 9.40 AM	**Indresh Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani-campus 333 031 (Rajasthan), India **Glutaraldehyde as suitable substrates for aminocatalytic annulation reactions: Synthesis of medium sized *N*-heterocyclic compounds**
IL-45 9.40 AM - 10.00 AM	**Hitendra. M. Patel** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar-388 120, Gujarat, India **Green chemistry concepts and its role for sustainability towards the development of Multi-component reactions**
O-18 10.00 AM - 10.10 AM	**Anubhuti Jha** Department of biotechnology, National institute of technology Raipur, Chhattisgarh, India

	Natural products based cinnamic acid scaffoldfor novel antifungal drug discovery against *Candida albicans*
O-19 10.10 AM -10.20 AM	**Vivek Gupta** Tata Institute of Fundamental Research, Centre for Interdisciplinary Sciences, Hyderabad-500075, India **Mono and Dinuclear Cyclic Six-membered Palladium Complexes Derived from Palladium Mediated C-N Coupling of Organonitrile and Formamidine: Synthesis, Structure, Reactivity and Catalytic Activity**
O-20 10.20 AM -10.30 AM	**Chandra Pal Singh** Department of Botany, University of Rajasthan, J. L. N. Marg, Jaipur-302004, Rajasthan, India **MicroRNAs as mediators of viral evasion of the host immune system**
O-21 10.30 AM -10.40 AM	**Amit Rajput** Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208 016, India **[CoIII(L)2]z Complexes (L = Azo-appended *o*-Aminophenol; z = 1–, 0, 1+, 2+). Ligand Redox-Level Mixed-Valency in the Neutral Form**
O-22 10.40 AM -10.50 AM	**Wahid M. Basyouni** Organometallic and organometalloid Chemistry Dept., National Research Centre, Dokki, Cairo, Egypt **SYNTHESIS AND EVALUATION OF ANTIVIRAL ACTIVITY OF SOME NOVEL HYDROXYBENZYLIDENE THIOSEMICARBAZONE DERIVATIVES BY USING BOVINE VIRAL DIARRHEA VIRUS AS A MODEL OF HEPATITIS C VIRUS**
O-23 10.50 AM -11.00 AM	**Prasanta Kumar Hota** Department of Chemistry, School of Sciences, Hemvati Nandan Bahuguna Garhwal University, Srinagar (Garhwal) – 246 176, India **Conjugated Molecule : Substituent directed light induced properties and medicinal activities**
O-24 11.00 AM -11.10 AM	**Sangiliyandi Gurunathan** Department of Stem Cell and Regenerative Biotechnology, Konkuk University, Seoul 143-701, Republic of Korea **GRAPHENE OXIDE SILVER NANOPARTICLES NANOCOMPOSITE: A MULTIFUNCTIONAL MOLECULES**
O-25 11.10 AM -11.20 AM	**Himadri Acharya** Centre for Soft Matters, Department of Chemistry, Assam University, Silchar-788011, Assam, India **Layered double hydroxide/ metal organic framework nanocomposites for adsorptive removal of anionic dye**
O-26 11.20 AM -11.30 AM	**Santosh Kumar** Department of Organic and Nano System Engineering, Konkuk University, Seoul 05029, Korea **Enhanced CO_2 capture of chitosan-zeolite composites for environmental applications**
11.30 AM - 11.40 PM	**Tea**

Parallel Session – VIII A

Chairpersons: Dr. A.K. Dwivedi, Dr. Vinay Tripathi

O-27 11.40 AM -11.50 AM	**M. P. Somashekarappa** Departmrnt of PG Studies in Chemistry, IDSG College, Chikkamagaluru, Karnataka state, India **Electrodeposition of polythiophene on self assembled molecular films of mercapto and methyl mercapto derivatized terthiophene**
O-28 11.50 AM -12.00	**Ashok Garai** Department of Physics, The LNM Institute of Information Technology, Sumel, Jaipur 302031, India **Pulling of DNA: Emergence of new structural polymorphs and S-DNA**
O-29 12.00 -12.10 PM	**Saeikh Zaffar Hassan** Department of Petroleum Studies, Z. H. College of Engineering and Technology, Aligarh Muslim University, Aligarh, India **Method Developed through Design of Experiments (DOE) for the Prediction of Rate Constant and Reaction Kinetics**
O-30 12.10 PM -12.20 PM	**Gitanjali B. Shelar** Assistant Professor, Department of Botany, School of Science, Sandip University, Nashik-422213, Maharashtra, India **Detection of Antagonistic properties of different fungus synthesized silver nanoparticles against Gram negative bacteria's**
O-31 12.20 PM -12.30 PM	**Anusaya S. Chavan** Department of Chemistry, Dr.BabasahebAmbedkarMarathwada University, Aurangabad, India **A facile synthesis of tetrahydrobenzo[*a*]xanthene-11-ones accelerated by whole cell biocatalyst, Baker's yeast**
O-32 12.30 PM -12.40 PM	**Anuj K. Sharma** Department of Chemistry, Central University of Rajasthan, NH-8, Bandarsindri, Ajmer, Rajasthan, 305817, India **Congo-Red-inspired-azo-stilbene molecular frameworks designed for metal-chelation therapy in Alzheimer's disease**
O-33 12.40 PM -12.50 PM	**Anjali Patel** Department of Chemistry, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390002, Gujarat, India **Invitro release study of Camptothecin from functionalized Mesoporous silica materials**
O-34 12.50 PM -1.00 PM	**Khushtar A. Salman** Department of Biochemistry, J.N. Medical College, Aligarh Muslim University, Aligarh, U.P., India **Prolonged exposure to industrial pollutants induce oxidative stress in humans**
O-35 1.00 PM -1.10 PM	**Idhayadhulla Akbar** Research Department of Chemistry, Nehru Memorial College (Affiliated to Bharathidasan University), Puthanampatti-621007, Tiruchirappalli (Dt), Tamil Nadu, India **Design and synthesis of linoleic acid peroxidation inhibitors of morpholine-**

	connected pyrazolidine derivatives induced by effective antimicrobial activity
O-36 1.10 PM -1.20 PM	**Parnas S. Parmar** Department of chemistry, Veer Narmad south Gujarat University, Udhana-Magdalla road, Surat - 395007, India **Synthesis and Biological evaluation of pyrazolopyrimidine and pyrazolopyridine derivatives**
O-37 1.20 PM -1.30 PM	**Sada Venkateswarlu** Department of Nanochemistry, Gachon University, Seongnam 13120, Republic of Korea **Fe_3O_4 Embedded NH_2-MIL 125 (Ti) MOF Composite for Selective and Efficient Removal of Aqueous Lead**
1.30 PM - 2.00 PM	**Lunch**

Parallel Session – VIII B

Chairpersons: Dr. Rajender Dahiya, Prof. Lalita Ledwani

IL-46 11.40 AM -12.00	**D. N. Singh** Department of Chemistry, K.S. Saket PG College, Dr. RML Avadh University, Faizabad- 224001, India **New Triterpenoid from the Aerial Part of *Phlebophyllum kunthianum***
O-38 12.00 -12.10 PM	**Ruby Singh** Department of Chemistry, School of Basic Sciences, Jaipur National University, Jaipur, Rajasthan, India **GREEN SYNTHESIS OF NOVEL SPIRO NITROGEN AND SULFUR CONTAINING HETEROCYCLES AND THEIR ANTI-INFLAMMATORY ACTIVITY**
O-39 12.10 PM -12.20 PM	**Masrat Maswal** Department of Chemistry, Government Degree College Boys,Pulwama, 190008, India **Rheological behavior and Ibuprofen delivery applications of pH responsive composite alginate hydrogels**
O-40 12.20 PM -12.30 PM	**Akhil Agrawal** Energy and Environment Research Laboratory, Department of Microbiology, Central University of Rajasthan, Ajmer, India **An Effective Approach for Enhanced Recovery of Oil using Polymer-Nickel Nanoparticles Mixture**
O-41 12.30 PM -12.40 PM	**Shikha Jain** Department of Chemistry, Manipal University Jaipur, Jaipur, Rajasthan, India **Natural sunscreen development from cyanobacterial isolates of hypersaline environments of India**
O-42 12.40 PM -12.50 PM	**Ibrahim, M. B** Department of Pure and Industrial Chemistry, Bayero University, P.M.B. 3011, Kano, Nigeria **Green Synthesis of Zinc Nanoparticles using *Ipomoea asarifolia*Leaves Extract**

	and its Application for Dyes Removal
O-43 12.50 PM -1.00 PM	**Rupasree Choudhury** Department of Chemistry, National Institute of Technology Agartala, Agartala, Tripura-799046, India **Study of Aggregation Kinetics of Macrocyclic Polyammonium Cations Guided Aggregation of Citrate Capped Silver Nanoparticles**
O-44 1.00 PM -1.10 PM	**Minu G Bhowon** Department of Chemistry, Faculty of Science, University of Mauritius, Reduit, Mauritius **Synthesis and biological properties of palladium complexes**
O-45 1.10 PM -1.20 PM	**Tenimu A. Abubakar** Chemistry Department, Sule Lamido University, Kafin Hausa, PMB 048, Jigawa state, Nigeria **Synthesis and characterization of substituted Mo and W carbonyl complexes containing isoniazid and dimethylglyoxime**
O-46 1.20 PM -1.30 PM	**Anusha Subramanian Mohanakrishnan** Chemical Engineering Department, Central Leather Research Institute (CLRI)1, Adyar, Chennai 600020, Tamil Nadu, India **Thermokinetic of poly(3-hydroxybutyric acid)(PHB) batch production by Azotobactervinelandii**
1.30 PM - 2.00 PM	**Lunch**

Parallel Session – IX A

Chairpersons: Prof. M. S. Shingare, Dr. Tanmoy Chakraborty, Prof. D. V. Mane

IL-47 2.00 PM -2.20 PM	**N C Desai** Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002, India **Fluorine Chemistry–An important tool for new drug discovery program in the 21st century**
O-47 2.20 PM -2.30 PM	**Sonia Nain** Department of Chemistry, Deenbandhu Chhotu Ram University of Science and Technology, Murthal, Sonepat - 131 039, Haryana, India **SYNTHESIS AND EVALUATION OF SOME NEW COMPLEXES OF 6-METHOXY-3FORMYLCHROMONE WITH COPPER (II), COBALT (II) AND ZINC (II) AS POTENTIAL ANTIMICROBIAL AGENTS**
O-48 2.30 PM -2.40 PM	**S. M. Gumel** Department of Pure and Industrial Chemistry, Bayero University, Kano - Nigeria **EXTRACTION OF CELLULASE ENZYME FROM TOMATO FRUITS AND PINEAPPLE PEEL USING *ASPERGILLUS NIGER* AND ITS APPLICATION IN TEXTILE WET PROCESSING**
O-49 2.40 PM -2.50 PM	**Aminu A. Umar** Department of Biochemistry, Kebbi State University of Science and Technology, Aliero, P.M.B 1144 Birnin Kebbi, Nigeria

	Cooperative regulation of human Exonuclease1 (hExo1) activity by 14-3-3 proteins
O-50 2.50 PM -3.00 PM	**Surajbhan Sevda** IIT Guwahati, Guwahati, India **Removal of nitrogenous pollutants and organic matters simultaneously from two different wastewaters using biocathode microbial fuel cell**
O-51 3.00 PM -3.10 PM	**Naveen Kumar Singh** Environmental Science discipline, Department of Chemistry,Manipal University, Jaipur-303007, India **PLANT-METAL INTERACTIONS FOR SOIL AND WASTEWATER TREATMENT**
O-52 3.10 PM -3.20 PM	**Garba Alhaji Adamu** Department of Science Laboratory Technology, Kano State Polytechnic, Nigeria **HEAVY METALS POLLUTION OF SURFACE WATER AND SEDIMENT OF WATARI RESERVOIR, KANO STATE, NIGERIA**
O-53 3.20 PM -3.30 PM	**Islam Khan** Biochemistry Department, Faculty of Medicine, Kuwait University, Kuwait **Uncoupling of Na-H Exchanger-1 and Carbonic Anhydrase in Inflamed Colon in Experimental Colitis**
O-54 3.30 PM -3.40 PM	**S. Jhaumeer Laulloo** Department of Chemistry, Faculty of Science, University of Mauritius, Reduit, Mauritius **The potential application of aromatic and cyclic amino acid based surfactants in soap-like formulations**
O-55 3.40 PM -3.50 PM	**Surendra Nimesh** Central University of Rajasthan, India **Nanomedicine based strategies for the treatment of Hypercholesterolemia and related Cardiovascular diseases**
3.50 PM - 4.00 PM	**Tea**

Parallel Session – IX B

Chairpersons: Dr. Nitu Bhatnagar, Prof. Sangeeta Jha

IL-48 2.00 PM -2.20 PM	**Rajeev Sakhuja** Department of Chemistry, Birla Institute of Technology and Science, Pilani 333031, Rajasthan, India **Functionalized Heterocycles as Biologically active Pharmacophores and Organic Materials**
O-56 2.20 PM -2.30 PM	**Vaibhav P. Mehta** Department of Chemistry, Faculty of Science, Marwadi University, Gauridad, Rajkot - Morbi Highway, Rajkot, Gujarat, India **Ruthenium-Catalyzed Cascade C-H Functionalization of Phenylacetophenones**
O-57	**Ranjan Khunt**

2.30 PM -2.40 PM	Department of Chemistry, Saurashtra University, Rajkot, Gujarat, India **Synthesis of novel imidazo[1,2-a]pyridine-4-hydroxy-2H-coumarins by GBB multicomponent reaction aspotential NS5B inhibitors**
O-58 2.40 PM -2.50 PM	**Sabir Hussain** Department of Chemistry, GGDSD College Palwal (M.D University Rohtak), Haryana 121102, India **SYNTHESIS, CHARACTERIZATION AND PHARMACOLOGICAL ACTIVITIES OF SOME SUBSTITUTED HETEROCYCLIC COMPOUNDS**
O-59 2.50 PM -3.00 PM	**Meenakshi Pilania** Department of Chemistry, Birla Institute of Technology and Science, Pilani-333031, Rajasthan, India **Triazolium ion Based *N*-Heterocyclic Carbene Precursors: Efficient Synthesis and Photophysical Properties**
O-60 3.00 PM -3.10 PM	**Manoj Lakhan** Deptt.of Physics, M.L.V. Govt.College Bhilwara Rajasthan, India **The Effect of Temperature on Photovoltaic (PV) Efficiency**
O-61 3.10 PM -3.20 PM	**KANTA MEENA** Department of Botany, M. L.V. Government College, Bhilwara - 311 001, Rajasthan, India ***BALANITES AEGYPTIACA* (LINN.) DELILE USED AS VETERINARY MEDICINE BY MEENA TRIBE OF TONK DISTRICT OF RAJASTHAN**
O-62 3.20 PM -3.30 PM	**Devesh S. Agarwal** Department of Chemistry, Birla Institute of Technology and Science, Pilani 333031, Rajasthan, India **Aggregation-Induced Emission Enhancement (AIEE): A Rationale for "Enzyme-Free" Detection of Cholesterol**
O-63 3.30 PM -3.40 PM	**Om P. S. Patel** Post-Doc Fellow, Chemistry Department, BITS Pilani, Pilani Campus, Rajasthan, India ***In vitro* and *in vivo* antidiabetic activity of carbazole alkaloids and their pharmacokinetic study**
O-64 3.40 PM -3.50 PM	**Sridhar S. N. C.** Department of Pharmacy, Birla Institute of Technology and Science Pilani (Pilani Campus), Pilani - 333 031, Rajasthan, India **Synthesis, Evaluation and Molecular Modelling Studies of 2-(Carbazol-3-yl)-2-oxoacetamide Analogues as a New Class of Potential Pancreatic Lipase Inhibitors**
3.50 PM - 4.00 PM	**Tea**

4.00 PM - 5.00 PM	**Valedictory Session**
5:00 PM – 5:30 PM	**ISCB General Body**

PLENARY

PL-1

Marine Alkaloid Analogs Inhibit Kinases and Growth of Cancer Stem Cells

Girolamo Cirrincione

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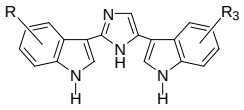
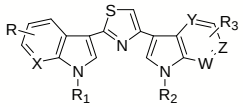
Marine organisms constitute a very unique source of bioactive molecules belonging to a great variety of different chemical structural classes. Among marine derived bioactive molecules, over 70 novel compounds showed significant inhibitory activity against kinases, important enzymes involved in vital role cell regulation and signal transmission pathways, controlling cell differentiation, proliferation and apoptosis.[1] Several marine derived molecules are in the pharmaceutical pipeline and have successfully reached the market. In particular there are six FDA-approved drugs and many others are under clinical trials.[2]

Bis-indole marine alkaloids, have emerged as important lead compounds for the discovery of new biologically active derivatives due to their potent biological activities shown. Among them, nortopsentins A–C having a characteristic 2,4-bis(3'-indolyl)imidazole skeleton, isolated from *Spongosorites ruetzleri*, exhibited in vitro cytotoxicity against P388 cells (IC_{50} values: 4.5–20.7 µm)and their synthetic analogsin which the imidazole moiety of nortopsentin was replaced by different 5-membered heterocycles, showed improved biological activity against a wide range of human tumor cell lines with GI_{50} values reaching sub-micromolar level. In particular, thiazole nortopsentin analogs**1-4**, in which one or both indole units of the natural nortopsentins were also manipulated, showed even better activity andinhibition of cyclin-dependent kinase 1 (CDK1).[3]Many derivatives, belonging to this class of compounds, revealed significant biological activity also in STO e MesoII cell lines,derived from human diffuse malignant peritoneal mesothelioma (DMPM), a very aggressive and resistant form of cancer,inducing a caspase-dependent apoptotic response, with a concomitant reduction of the expression of the anti-apoptotic protein survivin. The most active derivatives were also investigated *in vivo* showing a significant tumor volume inhibition of DMPM xenografts (range, 58%-75%) at well-tolerated doses, and two complete responses in each treatment group.



Nortopsentins



Thiazole Nortopsentin Analogs
1 X=Y=Z=CH, W=N; **2** X=W=N, Y=Z=CH;
3 X=N, Y=W=Z=CH; **4** X=Y=W=CH, Z=N;

In order toconfirm the therapeutic efficacy of this series of compounds, further studies were performed against cancer stem cells(CSCs) subpopulation freshly isolated from surgical resections of patients with the aim to identify new molecules potentially useful in therapy. Preliminary data showed that the treatment of colorectal CSCs, bearing different mutational background, with thiazole nortopsentin analogs, induced reduction of cells viability at 24 hours, potently induced the exit of CSCs from dormancy state. This phenomenon rendered the highly resistant CSCs sensitive to conventional chemotherapy drugs, oxaliplatin and 5FU. These results supported the use of these compounds as an innovative differentiation therapy that could be used in combination with standard chemotherapy as additive effect.

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PL-2

Synthesis of Regiospecifically Fluorinated Polycyclic Aromatic Hydrocarbons and Influence of Fluorine Atom

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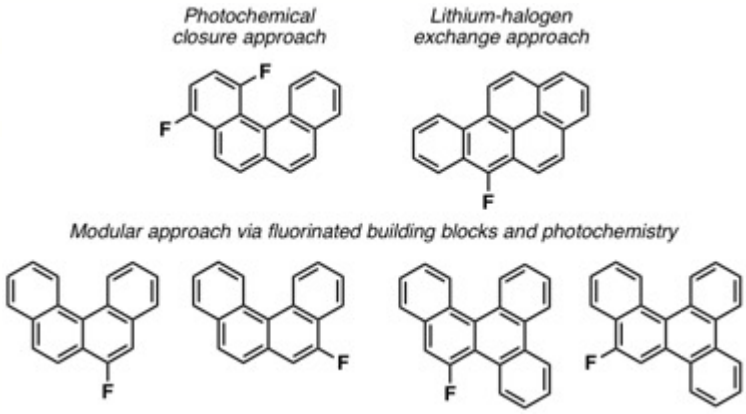
Replacement of hydrogen by fluorine atom can substantially influence physical, chemical, and consequently biological properties of molecules. Regiospecific introduction of fluorine continues to be challenging, despite active research in the area of organofluorine chemistry.[1] Fluorinated polycyclic aromatic hydrocarbons (PAHs) are of interest in diverse fields, ranging from materials, to environmental analyses, to studies in the area of chemical carcinogenesis. Synthesis of several regiospecifically fluorinated PAHs will be presented, and the effect of fluorine on shapes and/or biological activity and potential biologically important probes will be discussed.[2,3]



Acknowledgments

Support of this work by NSF Grant CHE-1565754and PSC CUNY awardsto BZis 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

S. Chandrasekhar

Director, CSIR-Indian Institute of Chemical Technology, Hyderabad, India

Abstract Awaited

PL-4

Understanding Retinal-Bound Photoreceptors through Bioorganic Chemistry

Anil K. Singh

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Sensory (*e.g.* vision) and energy (*e.g.* ion transport) transductions in several organisms ranging from bacteria to humans are powered by retinal-bound biological photoreceptor proteins, commonly called Rhodopsins. In spite of the diversity of occurrence in wide range of hosts, these photoreceptor proteins use a common ultrafast photoisomerization of their retinylidene Schiff base chromophore to store/transfer light energy, which is ultimately employed to drive protein's function *via* complex protein-chromophore interactions. Visual pigment Rhodopsin (Rh) is the prime example of such a photoreceptor, and which is the basis of animal vision. Bacteriorhodopsin (bR) found in the purple membrane of archaebacteria, *Halobacterium salinarium* is another photoreceptor of this type, which allows conversion of light energy into metabolic energy, required for vital functions of halobacteria. Because of their unique structural and functional features, these photoreceptors have become a paradigm for membrane-bound proteins in general, and sensory and energy transducer/transporters in particular. These photoreceptors have also attracted a great deal of attention in recent years because of their great potential in molecular electronic applications. Natural or laboratory-designed such photoreceptors have been successfully tried for development of opto-electronic devices, particularly holographic thin films and memory devices, optical information processing technology, retinal prosthetic device, and colour sensitive artificial retina, etc.. Our endeavour over the years has been to gain molecular insight into the general structure and mechanism of function of these photoreceptors through bioorganic approaches.

This talk, will elaborate upon how bioorganic models of bR were designed and used for developing an understanding of the structural and functional features of Rhodopsins. Our investigations have primarily contributed to build a molecular understanding of the protonation and stability of the retinyledene Schiff base chromophore and also to the colour control mechanism in Rhodopsins. The excited state studies of retinylidene and related linearpolyenes have led us to invoke the role for conformationally relaxed intramolecular charge transfer (CRICT) states in the photoprocesses of retinal-bound biological photoreceptors. This knowledge has also led us to develop neutral and hydrophobic fluorescent molecular probes based on CRICT-capable molecules, which find applications in the study of microenvironment of organized assemblies and proteins. The basic knowledge generated from these investigations has also enabled us to develop single- and multiple-cycle photoswitches. Thus, we could design several one-dimensional caging platforms and demonstrate that such phototriggers can be used for site, time and dose-controlled release of bioactive component from the cage under physiological conditions.

This talk while focusing on our efforts towards building molecular level understanding of the optical control of the structure and functions of Rhodopsins and related photoreceptors, and the challenges of molecular design of synthetic phototriggers and photoswitches along with their possible application scenarios, will also review the recent accomplishments in the field and highlight future inroads into other fields.

PL-5

Strategic Alkylations of Nitriles and "Isonitriles"

Fraser F. Fleming

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Metalated nitriles are nucleophilic chameleons whose structure is intimately tied to the nature of the metal counter ion, temperature, and solvent. Varying the environmental conditions provides selective access to an array of N-metalated nitriles, nitrile-stabilized carbanions, and C-metalated nitriles which have distinctly different structures and properties (Figure 1). The structural information will be used to explain how nitriles can be used for selective carbon-carbon bond formation: stereoselectivity, regioselectivity, chemoselectivity.

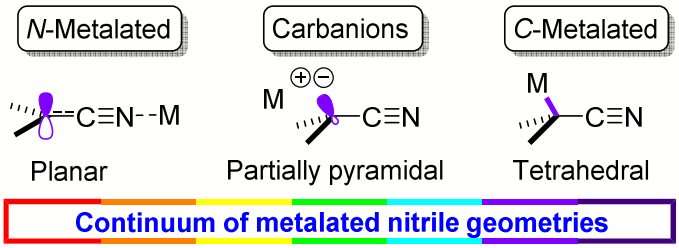

Figure 1

Although isoelectronic, metalated "isonitriles" or isocyanides are difficult to manipulate because thedeprotonation-alkylation is plagued byrapid self-condensation.Strategies to access metalated isocyanideswill be presented with an emphasis on ASMIC, **A**nisyl**S**ulfanyl**M**ethyl**I**so**C**yanide, an new isocyanide building block that provides access to a diverse array of trisubstituted isocyanides (Figure 2). ASMIC alkylations are high yielding, allow significant structural variation, with minimally odiferous intermediates to provide diverse isocyanides for applications such as heterocycle synthesis and multi-component reactions.

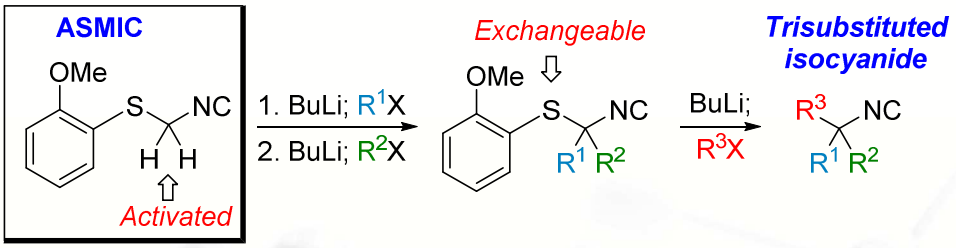

Figure 2

PL-6

(Diacetoxyiodo)benzene-Mediated Cyclization Reactions of N^6-Aryl and N^6-([1,1'-Biaryl]-2-yl) Adenosine Derivatives

Mahesh K. Lakshman

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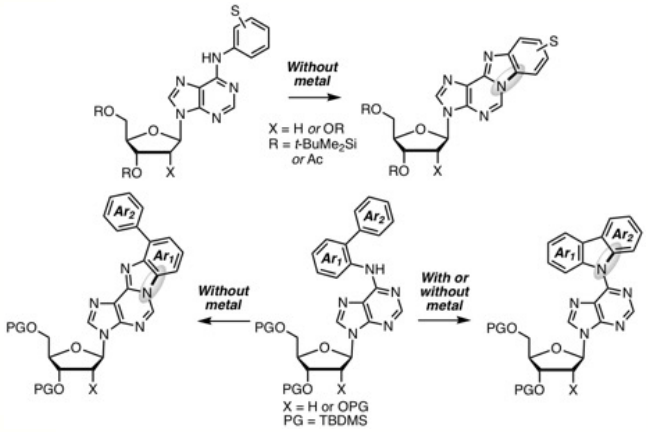
Access to N^6-aryl and N^6-([1,1'-biaryl]-2-yl) adenosine derivatives is readily available*via*either Pd-catalyzed C–N bond-forming reactions,[1,2]or by amide-activation reactions of inosine and 2'-deoxyinosine followed by S_NAr reactions with aryl amines.[3–5] These arylated compounds are well set up to undergo cyclization reactions with $PhI(OAc)_2$. The N^6-aryl adenosine derivatives undergo facile cyclization to benzimidazolyl purine nucleoside analogues,[6] but the N^6-([1,1'-biaryl]-2-yl) adenosine analogues undergo cyclization to carbazolyl nucleoside derivatives. Reaction conditions (Pd catalysis or uncatalyzed reactions in fluorinated solvents) and reaction solvents (fluorinated solvent *versus* acetonitrile) elicit significant influence on the outcomes from these reactions.[7] Mechanistic aspects have been evaluated as these reactions can partition *via* radical cations, nitrogen-centered radicals, and nitrenium ions.[6,7]



Acknowledgments

Support of this work by NSF Grant CHE-1265687 and PSC CUNY awardsto 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-7

Reversible Reservoirs for Radicals. A Powerful Strategy for the Creation of Carbon-Carbon Bonds

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Radical reactions offer many of the properties desired by synthetic organic chemists, in terms of variety, mildness of conditions, and a selectivity that is often complementary to that of ionic chemistry, making many protection steps superfluous. There is however one major difficulty, which derives from the propensity of radicals to interact with themselves (dimerisation, disproportionation) with extremely fast rates that are close to diffusion. In order to overcome this complication, it is essential to keep the steady-state concentration of radical species very low. This can be accomplished for example by contriving a chain reaction where the propagating steps are themselves quite fast, as for example in the typical, and now extremely popular, stannane based processes. While various *unimolecular* cyclisation and fragmentation steps can be efficiently incorporated into the radical sequence, kinetically slower *bimolecular* transformations, and in particular *intermolecular* additions to un-activated alkenes, have proven more difficult to implement. In the case of stannanes, the relatively slow addition to the alkene has to compete with premature hydrogen atom abstraction from the organotin hydride, a step that is usually thousands of times faster.

Over the years, we have shown that xanthates and related thiocarbonylthio derivatives allow the generation of radicals under conditions where the radicals possess a considerably increased effective lifetime even in a concentrated medium. Intermolecular additions to un-activated alkenes, as well as a variety of reputedly difficult radical transformations can now be easily accomplished. No metals, heavy or otherwise, are required, and the starting materials and reagents are cheap and readily available. Complex, densely functionalized structures can be constructed in a convergent, modular fashion. In the course of our study of the scope and limitations of this chemistry, we have uncovered a few surprising transformations. Recent results and some mechanistic aspects will be presented and discussed briefly.

PL-8

How RNase HI (E. coli) promoted site-selective hydrolysis works on RNA in duplex with carba-LNA and LNA substituted antisense strands in the antisense strategy?

Jyoti Chattopadhyaya

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

Abstract: A detailed kinetic study of 36 single modified AON–RNA heteroduplexes shows site-dependent modulation of RNase H promoted cleavage of complementary mRNA strands takes place at -GpN-3 cleavage sites, giving up to 70% of the mRNA cleavage products. A comparison of the modified AON promoted mRNA cleavage rates with that of the native AON shows that sequence-specificity is considerably enhanced as a result of modification. Clearly, relatively weaker -purine (Pu)–pyrimidine (Py)-stacking in the complementary RNA strand is preferred (giving 90% of total cleavage products), which plays an important role in RNase H promoted mRNA cleavage. A plausible mechanism of RNase H mediated cleavage of the mRNA will be presented. The enhancement of the total rate of cleavage of the complementary mRNA strand by up to 25%, presented in this work, provides opportunities to engineer a single modification site in appropriately substituted AONs to design an effective antisense strategy based on the nucleolytic stability of the AON strand versus RNase H capability to cleave the complementary RNA strand. Further Reading: Plashkevych, Li and Chattopadhyay, Molecular BioSystems (Royal SocChem/RSC) : Mol. BioSyst., 2017, 13, 921

PL-9

THIAZOLE AND THIAZOLIDINONE DERIVATIVES OF NATURAL ORIGIN AS ANTIMICROBIAL AGENTS

Victor Kartsev[1], Athina Geronikaki[2], , Marina Soković[4], Jasmina Glamočlija[4], Ana Ćirić[4]

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[4]*Institute for Biological Research "Siniša Stanković", University of Belgrade, 11000 Belgrade, Serbia.*

The treatment of infectious diseases remains an important and challenging problem mostly because bacterial infections have increased dramatically in recent years causing some of the most deadly diseases and widespread epidemics of human civilization .Through the past decades, the rapid progress of science led to the significant advances in the diagnosis and treatment of infectious diseases. Despite these efforts, the increasing number of multi-drug resistant microorganisms to known antibiotics, still keep the scientific interest in developing new classes of antimicrobial compounds. The problem of treatment infectious diseases became even greater taking into account the difficulties of dealing with the treatment of infections of hospitalized patients and protection of immunosuppressed and HIV-infected patients.

At the end of XX century about 80 percent of the world population to some extent are using natural compounds as medicines **[**1**],** pharmaceuticals of plant, vegetable or microbial origin make up more than 30% of global sales and about 70% of NCEs were obtained on the basis of natural products in 1981-2006 [2].

Taking all these into account in order to search for new representatives of antibacterial and antifungal compounds of the thiazole, thiazole and thiazolidine series, we screened several hundred compounds of these classes from the collection of InterBioScreen.

The representative structure is presented in Figure 1.

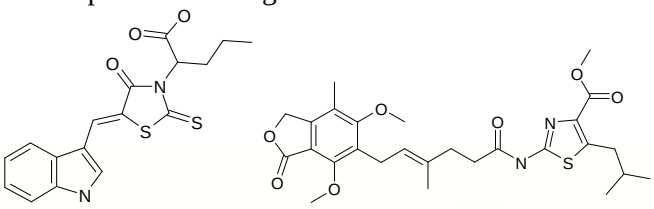

Figure 1. Structure of some of compounds tested.

Thus as a part of our ongoing studies in developing new active antimicrobials we describe herein the antimicrobial activity of selected compounds as well as their docking.

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PL-10

FROM MECHANISTIC UNDERSTANDING TO CATALYST APPLICATION: DEVELOPING NEW CATALYSTS FOR BOND-FORMING REACTIONS

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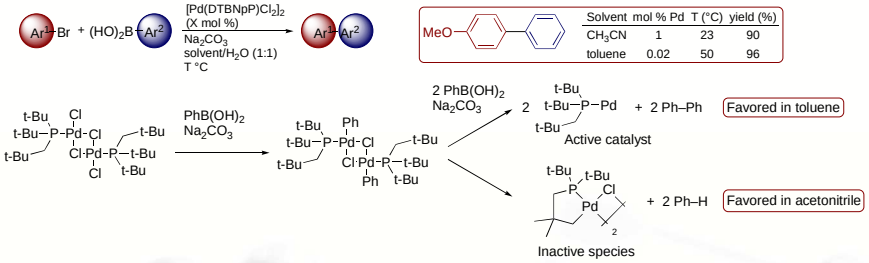
Homogeneous metal-catalyzed reactions play critical roles in the synthesis of biologically active molecules and pharmaceuticals. These powerful reactions have long played key roles in the drug discovery process and are increasingly being employed in process level syntheses. The development of high activity 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.[1]Recent research in the Shaughnessy group has focused on applications of conformationally flexible phosphine ligands. Phosphines with neopentyl substituents have steric demands comparable to tri-*tert*-butylphosphine, but in some cases are highly flexible and able to adopt smaller conformations. The highly flexible trineopentylphosphine ligand (PNp_3) affords catalysts that are highly active for the C–C and C–N coupling of sterically demanding substrates.[1e]Mechanistic study of this system shows that the rate of oxidative addition of aryl bromides to $Pd(PNp_3)_2$ is unaffected by the size of the aryl bromide.[1c]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.[2]Neopentylphosphines readily form palladacyclic complexes by C–H activation of the neopentyl substituent, which are inactive for cross-coupling of aryl bromides. The rate of palladacycle formation is strongly dependent on solvent polarity. By understanding this decomposition pathway the required catalyst loading for Suzuki cross-coupling could be lowered by a factor of 50 by changing the solvent from acetonitrile to toluene.The palladacyclic complex $[Pd(\mu\text{-}OAc)(\kappa^2\text{-}C,P\text{-}(t\text{-}Bu)_2PCH_2C(Me)_2CH_2)]_2$is effective for the cross-coupling of aryl alkynes with propargyl alcohol under mild conditions to afford 5-aryl-pent-4-yn-2-en-1-ol derivatives with high chemo-, regio-, and stereoselectivity.[3]



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PL-11

NOVEL THIAZOLIDIN-4-ONE DERIVATIVES WITH POTENT HIV-1 REVERSE TRANSCRIPTASE INHIBITORY ACTIVITY. DIVERGENCE FROM NON-COMPETITIVE INHIBITION MECHANISM

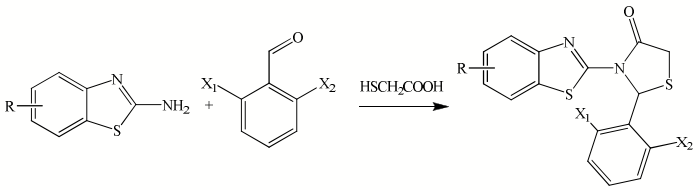
Athina Geronikaki, Eleni Pitta

Aristotle University of Thessaloniki, School of Pharmacy, Thessaloniki, 54124, Greece
e-mail: geronikaki@gmail.com

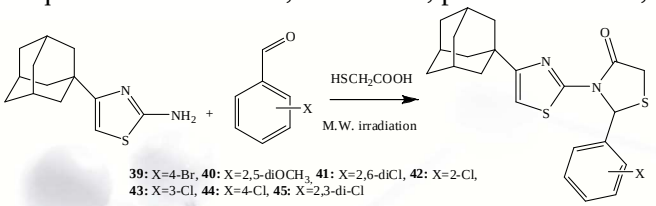
Human immunodeficiency virus (HIV) is a lentivirus that causes acquired immunodeficiency syndrome (AIDS), a condition in humans in which the immune system progressively fails and allows life-threatening opportunistic infections and cancers to thrive. Even if, 25 anti-HIV compounds have been formally approved for clinical use, no vaccine or cure is in sight. For this reason, there is an urgent need for the development of new therapeutic agents against HIV. Reverse transcriptase is one of the enzymes that play key role within the HIV replicative cycle and therefore it consists of the target of our research.

Based on the data from the literature regarding NNRTIs and taking into account the fact that cross-resistance is a common phenomenon, our aim is to design and synthesize new compounds, which preferentially exhibit a different mode of action, interacting with another part of RT. Two series of novel 4-thiazolidinones have been designed and synthesized, combining the thiazolidinone nucleus with benzothiazole or 4-adamantyl-thiazole groups, respectively.

Herein, we presented the synthesis and identification of 45 novel 2,3-aryl-thiazolidin-4-ones that could be divided into 2 groups: benzothiazole and 4-adamantyl-thiazole derivatives. All synthesized compounds were characterized by elemental analysis and spectroscopic methods (^{1}H NMR, ^{13}C NMR, HRMS).



Scheme 1. Reagents and conditions: (a) conventional method: toluene, reflux for 20–26 h, (b) microwave-assisted technique: absolute ethanol, 80–130 °C, power 50-200 W, 10–60 min.



39: X=4-Br, **40:** X=2,5-diOCH$_3$, **41:** X=2,6-diCl, **42:** X=2-Cl, **43:** X=3-Cl, **44:** X=4-Cl, **45:** X=2,3-di-Cl

Scheme 2. Reagents and conditions: microwave irradiation, absolute ethanol, 110–130 °C, power 100-200 W, 12–60 min

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PL-12

Olefin metathesis with modern ruthenium catalysts: applications in basic research and in industrial production

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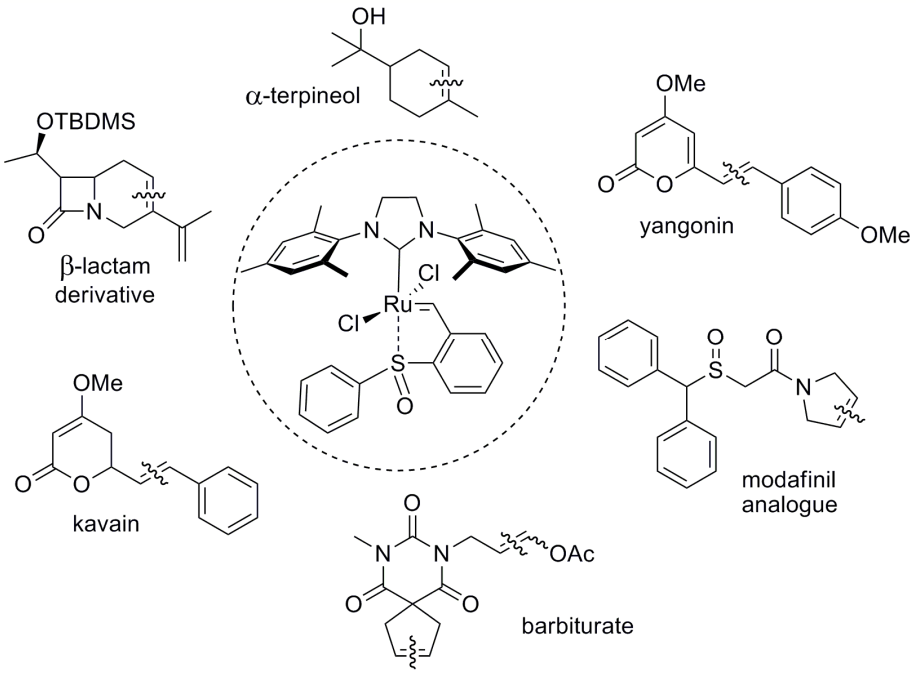
Ruthenium-catalysed olefin metathesis reactions represent an attractive and powerful transformation for the formation of carbon-carbon double bonds.[1] This area is now quite familiar to the most chemists as numerous catalysts are available that enable a plethora of olefin metathesis reactions, recently also in green solvents or without solvent.[1] However, immobilisation of the ruthenium alkylidene complexes, decreasing the amount of metal in products, using supported organometallic catalysts in medicinal chemistry,[2] nanofiltration, etc. still remain a challenge, making industrial applications of this methodology difficult.[3-5] These limitations can be solved *inter alia* by designing new, more active and stable catalysts that can be easier removed / recycled.



During the lecture a number of representative examples will be presented.

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INVITED

IL-1

Chemosynthetic Livers: Predict, Prepare and Prove the Structure, Activity and Toxicity of Drug Metabolites

Mukund S. Chorghade

We report advances in proprietary *in vitro* green chemistry-based technology, mimicking *in vivo* metabolism of several chemical entities used in pharmaceuticals, cosmetics, and agrochemicals. Biomimiks™ enables prediction of metabolism patterns and introduces new paradigms for drug discovery and drug-drug interactions for clinical diagnostics.

Metabolites are implicated in adverse drug reactions, and are the subject of intense scrutiny in drug R&D. Present-day processes involving animal studies are expensive, labor-intensive and chemically inconclusive.

Our catalysts (azamacrocycles) are sterically protected and electronically activated, providing speed, stability and scalability. We predict structures of metabolites, prepare them on a large scale by oxidation, and elucidate chemical structures. Comprehensive safety evaluation enables scientists to conduct more complete *in vitro* metabolism studies, confirm structure and generate quantitative measures of toxicity. Biomimiks™ is an animal-free platform that identifies a more complete set of safety-relevant drug metabolites while keeping up with the rapid pace of drug development.

Polypharmacy, involving co-administration of several drugs, is common among the elderly and chronically ill. It is a risk factor for adverse drug reactions (ADRs) and drug-drug interactions (DDIs). One plausible DDI occurs when a drug interferes with another, causing irreversible changes to formation of metabolites from one or both. Such suppression or attenuation of metabolism could cause variances in toxicity and efficacy. We report experiments to predict and confirm modulation of oxidative metabolites from several combinations of common drugs for cancer, diabetes, hypercholesterolemia and hypertension in the presence of each other. Recent papers indicate best evidence for the dimerization of some compounds in dilute aqueous solution or assorted complex formation between disparate compounds.

IL-2

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

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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-3

Development of Novel Polymeric Nanomaterials, Nanocomposites and Dendrons *via* Biocatalytic Routes

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We have developed a chemo-enzymatic synthesis for obtaining novel amphiphilic polymeric nanoparticles based on PEG having a broad range of additional chemical functionalities under mild conditions. Simplicity and versatility of this method for the synthesis of highly functionalized amphiphilic polymeric nanoparticles with the advantage of "Green appeal" further enhances its applications as an important strategy.

These unique alternating copolymer micellar **nanoparticles** have been used successfully for the encapsulation of a large number of drugs of different classes and delivery vehicles targeted to human cancer cells.

A novel nanotechnology platform for *in vivo* imaging and delivery of multifunctional thererapeutics of cancer has also been designed based on perfluorinated amphiphilic copolymers. These **nanoprobes** are highly unique because of their ability to image and treat the cancer tumors by delivering the drugs to the cancer tumor sites. Recently we have synthesized cationic polymers and **dendrons** that constitute of quaternary ammonium functional groups, polyglycerol and poly(ethylene glycol) units. The positive charge imposed on these macromolecules forms the basis for specific interactions between ligand and receptor or enzyme and substrate, *i.e.* as ammonium cations, they may bind to polyanionic DNA's and also to negatively charged cell surfaces to trigger endocytosis. Thus they may serve as gene siRNA delivery vehicles in order to cure many hereditary diseases and treat acquired diseases resulting from either multigenic disorders or foreign viral genes.

Further, highly useful novel, non-toxic "environment-friendly" non-halogenated flame retardant organo-silicone polymeric materials and nanocomposites have been developed using the above environmentally benign "green" biocatalytic technologies. These show superior properties than commercial flame retardant materials.

These results shall be presented in the talk.

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IL-4

Sugar Modification and Its Value Added Application

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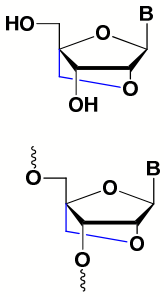
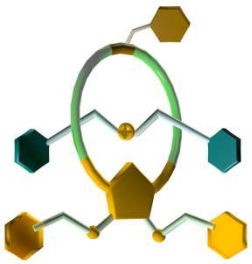
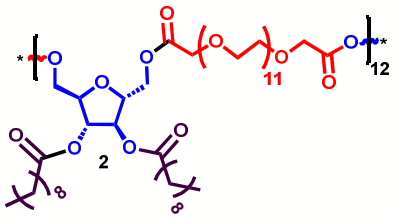
The use of biocatalysts in the modification of sugars has become an attractive alternative over conventional chemical methods due to their selectivity and high efficiency. We have successfully used lipases for the synthesis of sugar modified bicyclic nucleosides. Further, we have used the modified sugar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



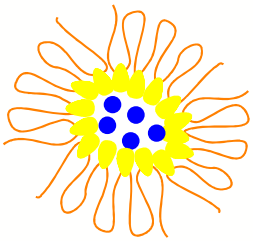




PEG 600

50 % acylation

C-10 alkyl chain



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

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IL-5

Asymmetric Synthesis of Izidine Alkaloids: Connection between Acetal and Hydroxylactam

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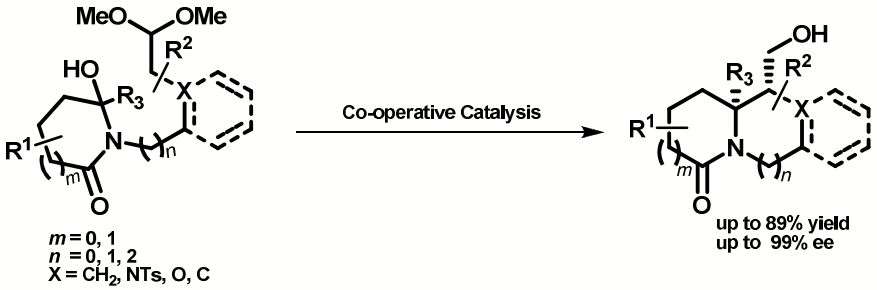
Abstract: Asymmetric organocatalysis[1] has been demonstrated as a powerful strategy for the synthesis of optically pure compounds from simple achiral precursors. Several otherwise impossible transformations have been documented in the last decade. Despite notable progress in implementing various transformations, 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-6

Exploration of protein motion, allostery, andintramolecular signaling of GPCR, and its implication in drug design

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Gprotein-coupled receptors (GPCRs)act as both gatekeeper and molecular messengers of the cell converting extracellular signals to cellular activities. Hence, elucidation of its allosteric modulation and related intra-molecular signaling would be of great help. To investigatethe allosteric regulation of GPCR, we adopted network centrality analysis to the apo and agonist-bound forms of A_{2A} adenosine receptor (A_{2A}AR). Through the analysis, we could precisely identify the location of micro-switches which are deemed critical for GPCR activation. Additionally, significant long-range communications were found to exist between the extracellular ligand binding site and G protein binding site in the agonist-bound form only.

Recently, we discovered novel modulators of A_3AR and identified minute chemical changes crossover the boundary between agonistic and antagonistic effects. To investigate this effect, new A_3AR homology models were constructed based on pharmacological profiles of the ligands. To account for the protein flexibility, the binding modes were predicted using multiple receptor conformations (MRCs). The results showed that the H-bonding with T94 is crucial for the agonistic effect of A_3AR. Interestingly, the network analysis also confirmed that T94 is important for signal flow in the receptor. Taken together, our structure-based studies using MRCs and network analysis can provide valuable insights into the allosteric modulation of GPCRs, and they could be utilized as a powerful tool in drug discovery.

IL-7

Monoisoamyl DMSA, a ray of hope for the treatment of Chronic Arsenicosis- Journey from lab to human trial

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Arsenic with low level chronic exposure acts as slow poisons with effects on possibly all organs to produce clinical and pathological signs and symptoms in human beings. There has been a major concern for the ever growing number of arsenicosiscases in India, Bangladesh, and other regions of South East Asia. Researchers across the globe have been working for the development of better clinical therapies using newer strategies and more effective drugs. Two important properties of conventional drugs that dictated the need for newer chelating agent and therapeutic strategies are i) side effects including non- specificity and inability to reach intracellular sites and 2) redistribution of metal. Moreover, randomized placebo trials conducted with US FDA approved drug (DMSA) further suggested that it is incapable of mobilizing arsenic from the tissues and hence did not provide clinical recoveries. This prompted our group to look for DMSA derivatives that would have similar chelating properties of DMSA and also lipophilic properties which would assist the chelator to gain intracellular access. A large number of esters of DMSA were synthesized and examined for achieving optimal chelation. Focusing on the potential chelator, they synthesized and utilized mono-isoamyl derivative of meso 2, 3-dimercaptosuccinic acid (MiADMSA, a C_5 branched chain alkyl monoester of DMSA) in various monotherapy and combinational therapies for the treatment of chronic and acute arsenic poisoning. They found the compound to be more effective than the parent compound (DMSA), in terms of eliminating the toxic metal and providing better clinical recoveries in animal models. The effectiveness of MiADMSA as a chelator was not just limited to removal of arsenic from the body but it also prevented other biochemical alterations. Various comparative studies reported the superior efficacy of MiADMSA compared to the parent compound in lowering arsenic burden from whole body and vital organs like kidney and liver. Our group validated the acceptability of MiADMSA as a potential chelator for the treatment of chronic arsenic poisoning. Drug Controller General of India has recognized this molecule as Investigational New Drug (IND) and gave permission for human clinical trials which are currently in progress.

IL-8

Neplanocin Derived Analogs: A potential scaffold as anti-HBV agents

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Abstract

The current therapy includes nucleoside analogs for Hepatitis B Virus (HBV) infection. Nucleoside analogs are potent inhibitors of HBV DNApolymerase (also acts as reverse transcriptase). The treatment is effective, however emergenceof drug-resistance and viral reactivation are major concerns in HBV. Thus, it is unmet need to develop novel inhibitors as curable drug for HBV infection. Neplanocin A (NPA,) is a carbocyclic nucleoside analog of adenosine with cyclopentene ring. It showed broad-spectrum antiviral activity, however failed to develop as a drug due to its cytotoxicity. In continuation to our nucleoside memetic design process, recently we reported that several neplanocin A derivatives for their inhibitory effect on HBV replication. Adenosine base modification showed some anti-HBV activity, which indicates the possibility to alter bioisosters of adenosine to enhance anti-HBV. In continuation to our neplanocin A (NPA) based antiviral research[1-2] using structure based approach provided a understanding that adenosine motif of NPA utilizing N-9 nitrogen and 4-amino group to bind with the active site of SAHase.[3] Thus, the two polar groups may be the major group for SAHase binding and need forbioisosteric replacement to avoid SAHase related toxicity. The bioisosteric replacement with methyl gave the interesting compound with significant antiviral activity[2]. Among neplanocin A derivatives, (1S,2R,5R)-5-(5-bromo-4-methyl-7H-pyrrolo[2,3-d]pyrimidin-7-yl)-3-(hydroxymethyl)cyclopent-3-ene-1,2-diol and (1S,2R,5R)-5-(4-amino-3-iodo-1H-pyrazolo[3,4-d]-pyrimidin-1-yl)-3-(hydroxymethyl)cyclopent-3-ene-1,2-diol were found to be selective inhibitors of HBV replication. Unlike neplanocin A, these compounds were not inhibitory to the activity of SAHase. These results suggest the discovery of NPA based analogs with new mechanism of action as anti-HBV agent. (Authors thanks to DST, India for financial support.)

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IL-9
(ISCB Best Teacher Award 2018)

Ionic hydrogenation-directed stereoselective construction of C-20(H) stereogenic center in steroid side chains: Scope and limitations

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Stereoselective synthesis of steroidal C-20 tertiary alcohols with 1,3-dithane, n-butyl, vinyl, furyl, thienyl, thiazolyl, aryl and pyridyl side chains via Grignard reaction or organolithium reagents have been realized starting from readily available 16-dehydropregnenolone acetate. The ionic hydrogenation of steroidal C-20 tertiary alcohols having 1,3-dithane, furyl, methylfuryl, thienyl, phenyl and 4-methoxyphenyl side chains, resulted into the deoxygenated product with C-20 natural/unnatural configuration in excellent yields. However, the alkyl, thiazolyl and pyridyl incorporated steroidal C-20 tertiary alcohols were failed under the same reaction condition. The scope of ionic hydrogenation is further highlighted through the stereoselective reduction of steroidal C-20,21-ene compounds with dithiane, furyl, thienyl and 4-methoxyphenyl side chains gave the saturated compounds with C-20 natural/unnatural configuration. The details will be discussed during presentation

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IL-10

Insights to the mechanistic pathway of tailored de novo antitumor Cu(II)/Zn(II) drug candidates: Structure elucidation and biological studies for validation of target sites

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Abstract:

New tailored **Cu(II)/Zn(II) drug** candidates involving the specific site of action at the target site possessing lower systemic toxicity were successfully synthesized and thoroughly characterized by single X-ray diffraction and other spectroscopic studies. Studying mechanistic insights or the precise pathway of cell inhibition is a challenging issue in the area of drug design**.**
Since targeted cancer therapy involves the use of small compounds/metallodrug candidates that block the growth and spread of cancerous cells by interfering with specific molecules or pathways that are involved in cancer growth or progression .It becomes mandatory to identify the types of targets at the molecular level, viz. nucleic acids (DNA and RNA), enzymes (kinase inhibitors and topoisomerases) and G-quadruplex DNA, pUC19 plasmid DNA, HCV SL II-b, SL IV, SF 16 RNA etc. We have carried out biological studies and molecular docking/DFT to validate these novel targets involved in various cancers phenotypes.

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IL-11

NON-COVALENT APPROACHES FOR THE DYNAMIC CONTROL OF DNA AND DNA-BASED MATERIALS

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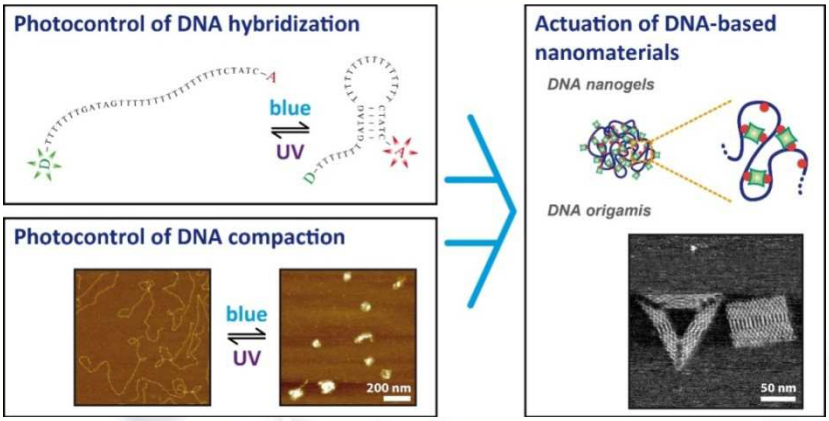
Even though the main natural biological function of DNA is the storage and transmission of genetic information, its specific chemical structure enables a wide range of *in vitro* applications spanning from biotechnologies to material sciences. In this talk I will present some of these applications, and especially the use of DNA as a brick for creation of new nanobiomaterials: DNA-protein conjugates [1], DNA nanogels [2] and DNA origamis [3]. I will also describe how to exploit the physico-chemical properties of DNA to create new ways to actuate these DNA-based nanomaterials. For this purpose we develop generic molecular tools able to affect and control two important DNA properties: compaction and melting, and this without any covalent modification of DNA. Compaction of DNA refers to the change of its higher-order structure upon electrostatic neutralization of the negative charges. I will show how this physico-chemical phenomenon can be used to control gene expression with light [4,5], modulate enzymatic activity of proteins conjugated to DNA [1], and induce the folding of bidimensional DNA origamis into surprising tubular 3D structures [6]. On the other hand, the melting of DNA corresponds to the separation of complementary strands upon heating and is opposite to DNA hybridization. In the second part of my talk I will describe a new class of molecules - photosensitive intercalators - able to stabilize DNA double helix in a photo-dependent manner. I will demonstrate the applications of these molecules to reversibly photo-induce the separation and re-hybridization of DNA strands at constant temperature not only in the case of linear double-stranded DNA, [7] but also for more complex DNA nanostructures, like DNA origamis, paving the way toward dynamic nanotechnologies.



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IL-12

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Abstract Awaited

IL-13

Metal Free Syntheses of Thioethers: Reactivity, Scope and Challenges

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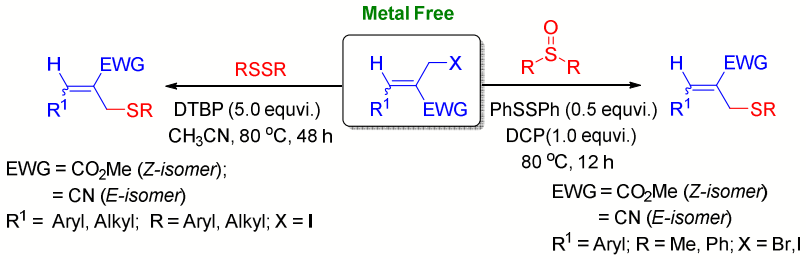
Abstract:

Due to environmental concerns and cost issues, the metal-free organic transformations are the need of hours. Enough progress has been made in this direction by using various catalytic systems in recent years,[1] the peroxide alone or with additives emerged as the perfect substitute to the traditional transition metal catalysis for several organic transformations.[2] Meanwhile, aryl thioethers have been found to playing important roles in organic synthesis, pharmaceutical industry and materials science. Recently, the syntheses of aryl thioethers have been reported under metal-free conditions *via* C-H functionalization using a variety of sulphur surrogates. Various catalyst or catalytic systems such as DTBP, TBHP, $K_2S_2O_8$, AcOOH, *etc.* have been so far used for the syntheses of thioethers *via* C-H functionalization.[3] In this talk, the recent advances in the syntheses of thioethers and thioesters under metal free conditions will be presnted.[3,4]



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IL-14

How Proteostasis Defects Contribute In Ageing And Neurodegeneration?

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Keywords: Proteostasis; *E3 ubiquitin Ligases; Ageing; Neurodegeneration; Chaperones*

Abstract:

In eukaryotic cells cellular protein quality control system uninterruptedly reduces deleterious accumulation of aberrant proteins. Ubiquitin proteasome system (UPS) specifically recognizeaberrant proteins for their degradation with the help of E3 ubiquitin ligases and regulates a central hub of an entire set of cellular expressed proteins. Chaperones promote protein folding and quality control (QC) E3 ubiquitin ligases careful clearance of aberrant proteinaceous inclusions to maintain proper cellular health and fitness. However, the precise molecular pathomechanism of misfolded proteins accumulation lead to neurodegeneration and ageing is not well understood. Previous findings indicate that lack of functions of E3 ubiquitin ligases may be a possible cellular factor of neurodevelopmental disorders, neurodegeneration, cancer and ageing. However, the detailed mechanism implying E3 ubiquitin ligases in cellular functions in multifactorial disease conditions are not well understood. Our present observations systematically represent the unique characteristics, molecular nature, and recent developments in the knowledge of neurobiological functions of selective crucial E3 ubiquitin ligases. It is important for us to understand that how modulation of few QC E3 ubiquitin ligases can serve as possible promising molecular therapeutic strategies linked with the fundamental challenges of proteostasis imbalance and thereby it may propose new lines of potential targets for therapeutic interventions.

IL-15

Assessment of Bioenhancing potential of Lysergol

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Abstract: Lysergol(LYZ), an indole alkaloid, is isolated from seeds of *Ipomoea muricata, I. turbinate* and *Calonyctionmuricata* [1]. It is intentionally used in formulations to increase the systemic availability of therapeutically active compounds [2-3].In the present study, the possible mechanism behind itsbioenhancingpotentialwas evaluated using curcumin (CUR;the principal curcuminoid from miracle Indian spice turmericcomprising ofplethora of medicinal capabilities that has low aqueous stability, poor absorption from the gut, rapid elimination and poor oral bioavailability [4])as model drug.

Initially,LC-MS/MS based bioanalytical methods were developed and validated for quantification of CUR, digoxin and sulfasalazine. First, the intestinal permeability enhancing potential of LYZ was evaluated by *in situ* single pass intestinal perfusion (SPIP) of CUR with and without LYZ co-perfusion. Then, *in vivo* pharmacokinetics of CUR (100 mg/kg, oral) was studied in male *Sprague Dawley* rats with or without pre-treatment with LYZ (20 mg/kg, oral).To investigate the mechanisticinsights, the *in vitro* phase Iand II metabolic stability studies of CUR following pre-incubation with LYZ using rat liver microsomeswere performed. Also, its effect on major efflux transporters using human P-gp andBCRP membrane preparations was examined using ATPase activity assay.For validation of transporter inhibition potential of LYZ, P-gp/BCRP ATPase activity was estimated by measuring the inorganic phosphate released from ATP.The observationswere compared with the inhibitory potential of verapamil (for P-gp) and pantoprazole (for BCRP).Intestinal perfusion and pharmacokinetics of digoxin (P-gpsubstrate) and sulfasalazine (BCRPsubstrate) were studied for further confirmation.

The LC-MS/MS methods showed adequate sensitivity, recovery, accuracy and precision for the intended purpose. In the presence of LYZ, the effective permeability (P_{eff}) of CUR was enhanced (3.3-fold), which infers that LYZ has a significant effect on $P_{eff}$of CUR. In rats, the C_{max} and elimination half-life ($t_{1/2}$) of CUR weresignificantly increased and the relative bioavailability of CUR was found to be 1607.3±419.8%. However, a noteworthy decrease in curcumin's clearance was observed that can be attributed to the intestinal and hepatic metabolic inhibitory action of LYZ.CUR (1 µM) showed remarkable decrease in its metabolism rate as the*in vitro* $t_{1/2}$ of CUR increased from 6 to greater than 60 min. The observations indicate a probability of inhibition of CUR glucuronidation in presence of LYZ.But, an insignificant change in the basal activity of membrane preparations containing P-gp indicates no or very less affinity of LYZ for P-gp. However, the significant increase in basal activity in presence of LYZ indicates its affinity for BCRP.Aninsignificant increase was observed in the P_{eff} of digoxin (P-gp substrate) in the presence of LYZ. These results are in strong agreement with the results obtained from ATPase assay indicating no role of inhibition of P-gp mediated efflux.The *in vivo*pharmacokinetic studies of digoxin with and without LYZ co-administration in ratsshowed an enhancedbioavailability of digoxin (increased AUC and decreased clearance of digoxin) but the increased bioavailabilitymay not be fully attributed to the inhibition of P-gp.On co-administration with LYZ, sulfasalazine showed a highly significant increase in AUC and was more noticeable than that foundin a well-established BCRP inhibitor (pantoprazole) co-treated rats.The ATPase assay and SPIP studies of sulfasalazine with and without LYZ provided strong evidence regarding the role of LYZ as a BCRP inhibitor.Theseobservations have demonstrated the bioavailability enhancing potential of LYZthatcan be credited to the inhibition of metabolic enzymes and BCRP efflux transporters.

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IL-16

Chemical Diversity of Benzimidazoles: Design, Synthesis, and Biological Applications

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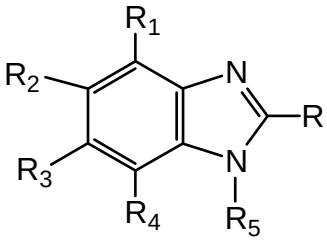
Benzimidazole is highly versatile heterocyclic ring system utilized in the therapeutics and wide-range of other applications has been developed.Chemically diversebenzimidazolesare designed based on the therapeutic target or applicationfrom simple substituted to more complex hybrid structures. In particular, novel benzimidazoles were synthesized and characterized for the biological applications of anti-aflatoxigenic, anti-bacterial, anti-fungal, and metal ion sensors.

In the presentation, one of the case studies of the structure-activity relationship (SAR) of 2-substituted benzimidazoles will be reported and investigated thoroughly for anti-fungal and anti-aflatoxigenic activities. However, the SAR of benzimidazoleshas found a lead compound for targeted inhibition of aflatoxin production without impacting the growth of fungi (*Aspergillus Flavus*). These findings could be utilized further in the food safety and beverages and brewing industries for controlling the aflatoxins. Also, several other applications of other benzimidazoles are highlighted in the presentation.



IL-17

The future of the PhD: A Careers Away from the Bench?

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As reported by the Survey of Earned Doctorates (SED), United States institutionsawarded more than fifty thousandresearch doctorate degreesin 2014. The number of doctorates awarded each year grow at an average rate of approximately three percentwith no sign of slowing. As per American Institutes for Research 2014 report, more than sixty percent of science, technology, engineering, and math (STEM) PhDs were working in nonacademic careers and thirteen percent of STEM PhDs had left these disciplines altogether. Increasingly, Ph.D.-level scientists are searching for career opportunities beyond bench research. The striking difference between the number of graduate students and postdocs, and the limited availability of tenure-track faculty positions means that nonacademic positons are no longer "alternative" career options. Most graduate students see post doctorate as their only option due to lack of information about other job opportunities. Here, we will discuss how to increase awareness about non-research based “alternative” career options.

IL-18

SILYL DIAZOENOLATES AS NUCLEOPHILES IN VISIBLE LIGHT PHOTOREDOX CATALYZED MANNICH REACTION

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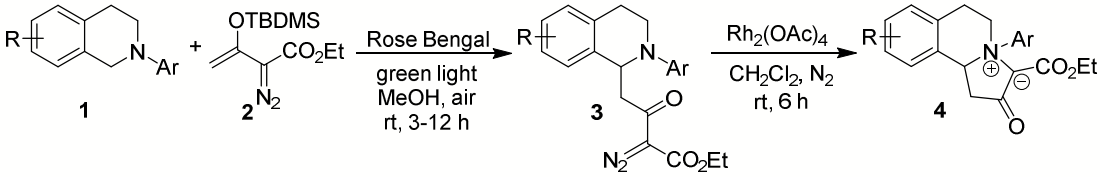
The α-functionalization of tertiary amines by activation of sp^3 C-H bonds adjacent to nitrogen is a powerful strategy for the synthesis of functionalized amines.[1] Out of various methods known for the α-C-H activation of tertiary amines, the most widely used one is oxidation of the amine into a reactive iminium intermediate which is then trapped by a suitable carbon or heteroatom nucleophile.[2] Recently, visible light mediated α-CH functionalization of tertiary amines employing organic dyes, Ru/Ir complexes, inorganic semiconductor photocatalysts or under sequence/dual catalysis has helped in the development of novel transformations of tertiary amines.[3] With enormous progress in terms of catalysts, oxidants and reaction conditions, the search for hitherto unknown nucleophiles has become even more vigorous.

Diazo compounds have been extensively utilized as nucleophiles owing to the nucleophilicity of their α-carbon.[4] Despite this there are only two reports for α-CH functionalization of tertiary amines with α-diazocarbonyl compounds.[5]

The present work documents the α-C-H functionalization of tertiary amines **1** via visible light catalyzed Mannich reaction with silyl diazoenolates **2**. The reaction takes place at room temperature with the organic dye Rose Bengal as a photocatalyst and oxygen as the oxidant. The resulting multifunctional products **3** bearing α-diazo-β-keto group undergo Rh-carbenoid mediated cyclization, affording stable ammonium ylides **4** in high yields.[6]



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IL-19

Carbonaceous fractions in Indoor Air Due to Burning Activities: Threat to Health and Climate

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ABSTRACT

The studies associated with carbonaceous particulates in indoor environment are the latest thrust research area. The carbon fractions generated out of various burning activities is serious threat to health and climate change. Carbonaceous aerosols (fractions) are the important components of smoke from household fuel burning, which has been contributing to the degradation of indoor environments and also have adverse effects on human health due to presence of toxic organic compounds, such as polycyclic aromatic hydrocarbons (PAHs) (and their alkylated homologues), which are proven carcinogens and mutagens. In addition to health effects, carbonaceous fractions have prominent implications for regional carbonaceous aerosol load in air (Jacobson, 2004) and seriously affect atmospheric radiation balance, which, in turn, could change regional rainfall patterns. Therefore, it is major concern of to investigate indoor emissions of smoke from household fuel burning in urban & rural residential households.

In urban areas, 70% of airborne fine particles are a result of combustion emissions and 50% are due to primary emissions from combustion sources. Combustion produces two, classes of nanoparticles with mean diameters of ~10 nm and ~1 nm. The impact of indoor solid fuel smoke brings it to 10th (~1.5 million premature deaths/year) as a risk factor for the global burden of disease, compared to active tobacco smoking, which is rated fourth (4.9 million deaths/yr) (WHO,2002). Acute lower respiratory infection (ALRI) (Smith *et al.*2004). ALRI is the single greatest cause of death of the world's children (>2 million/year), The other major disease that closely associates with these exposures is chronic obstructive pulmonary disease (COPD) in adult women, a major source of morbidity and premature mortality globally (Bruce *et al.*2000).

In India such studies have been conducted in various cities and rural areas, which establishes correlations that burning activities at all levels are responsible for regional climate changes and health effects.

IL-20
(ISCB Best Teacher Award 2018)

Nature-inspired Chemical Design and Efficient Syntheses of Drug-like Nitrogen Heterocycles

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Nitrogen heterocycles are among the privileged motifs that play vital roles in natural products and therapeutic agents endowed with antiproliferative activities. Identification of new chemotherapeutic agents for the treatment of cancer affliction is one of the leading areas in drug discovery (1). Most of the known anticancer agents are found to possess undesirable actions such as reduced bioavailability, toxicity, and drug resistance. Therefore, hunt for potent and selective anticancer agents are highly desirable. In line with this objective we have been investigating potent anti-proliferative agents containing indole, carbazole and porphyrin scaffolds. Developing mild, economical and scalable synthetic strategies to obtain valuable heterocycle-based agents are enduring challenges and immense scope for organic chemists. To prepare bioactive heterocycles, we have been using synthetic strategies like C-H functionalization, oxidative cyclization, click chemistry and metal-free direct arylation. Recently, we have demonstrated the synthetic utilities of organoiodine reagents to access 2-arylindoles, heteroaryl carboxylates, *N(O)*-arylquinolones, fused triazoles, oxazoles, oxadiazoles, thiadiazoles, natural products (Pallulone and Glycosinine) and drug analogues of Tafamidis and Boscalid (2). Our recent results related to chemical design and strategies to access drug-like heterocyclic molecules will be shared during the presentation.

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IL-21

Transition-metal catalyzed novel and sustainable strategies for the synthesis of bioactive heterocycles

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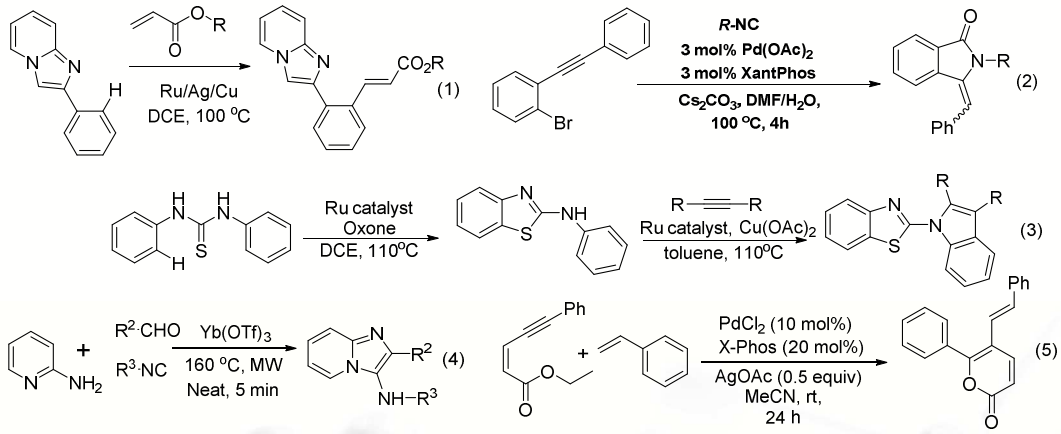
Heterocycles have wider and useful applications in many products that are used daily, ranging from pharmaceuticals, cosmetics, dyes, preservatives and LEDs. [1]Developing new and sustainable synthetic routes for generating diversified heterocycles in fewer steps is the latest horizons for the explorations in modern synthetic chemistry. Transition-metals play an pivotal roles as catalyst in these transformations. The development of efficient catalytic systems for various synthetic approaches such as C-H activation, isocyanide insertion, multicomponent reaction etc is a long-desired goal of chemists, as they provide environmental friendly and waste-reducing alternatives to classical methodologies for C−C and C−heteroatom bond formation. The main aim of our research at Central University of Rajasthan is to focus our attention on the application of transition metal catalyzed C-H activation[2] or multicomponent reactions[3] for the synthesis of diversified heterocyclic scaffolds. We successfully demonstrated Ru-catalyzed direct C-H activation for functionalization of 2-phenylimidaopyridines [Eq 1],[1a] cyclization of benzothiazole[1b]and benzothiazole directed oxidative annulation of anilines with alkyne [Eq 3].[1c]Similarly, isocycanide based multicomponent approachessuch as Palladium-catalyzed synthesis of diverse isoindolin-1-one derivatives via tandem Carboxamidation/Hydroamidation reaction [Eq 2],[2a]Ytterbium triflate-mediated rapid and quantitative synthesis of imidazo[1,2-a]pyridine [Eq 4],[2b]have been developed. Recently we demonstrated an efficient one-pot protocol for the synthesis of multi-substituted 2-pyrone derivatives from internal alkynes and unactivated alkenes [Eq 5].[2c]A complete depiction of these inventions will be presented.



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IL-22

Invention of A New Molecule RISUGadv in India for the Prevention of Prostate Cancer

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Abstract

Cancer is a dangerous disease that affects the regulation of cell cycle. Normal cell is converted into cancer cell by the serial mutations in its genetic material that exhibits uncontrolled proliferation. Prostate cancer is a type of cancer that basically affects the whole reproductive system, Prostate cancer is the second most common cancer in men worldwide. RISUGadv is a new molecule that will be used for the prevention of prostate cancer which was invented by Prof S. K. Guha at IIT, Kharagpur. This molecule is made up by the polymerization of styrene maleic anhydride and dimethyl sulfoxide.

CDRI is one of the most important institute in India in the area of drug discovery and development. The toxicity study of RISUGadv was done at this institute. The 14th days and 28th days toxicity study and genotoxicity study of RISUGadv was also done in this institute.The compound RISUGadv was also found safe in all systemic toxicity studies and no adverse effects were observed in any parameters related to toxicity study. In special toxicity study a set of experiment was conducted for the assessment of genotoxicity eg. AME's Assay, Chromosomal aberration assay, Micronucleus assay.

Key words:- RISUGadv, Prostate Cancer, Genotoxicity, Toxicity study.

IL-23

LC-MS/MS methods to identify characterize and determine bio active phytochemicals and study their variation in *Indian Medicinal Plants*

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Herbal medicines widely used in health-care in both developed and developing countries are complex chemical mixtures of medicinal plants. The use of herbal medicines has increased remarkably in line with the global trend of people returning to natural therapies. Standardization of herbal formulations is essential in order to assess the quality of drugs, based on the concentration of active principles present therein. Quality evaluation of herbal preparation is a basic requirement of organizations dealing with Ayurvedic and herbal products. The advent of modern synthetic medicines has brought with it unwanted side effects. Hence herbal medicine has now developed as a valid alternative system of therapy involving herbal formulations, supplements and functional foods. Modern analytical methods play an important role in the characterization and quantification of the phytoconstituents and hence in the standardization of herbal extracts and formulations. Applications of HRMS and LCMS/MS instruments will be discussed to characterize bioactive molecules and determine their quantity in different plant parts of Phyllanthus spp and Adhatoda spp.

IL-24

Plasma for Chemistry and Biology Interface

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Plasma is the forth state of matter, and defined as, conductive assemblies of charge particles, neutral particles, which exhibit collective behavior. Due to its collective behavior, it is an aggressive state of matter that contains energy and can be utilized for many biological applications. The chemistry of the plasma plays an important role in most plasma processing systems. The plasma processing application ranges from non-thermal to thermal plasmas. In non-thermal plasma applications the active species of plasma play an important role whereas in thermal plasma applications the higher temperature properties of the plasma control the chemistry. For most biological applications non-thermal plasmas are best suited. CSIR-CEERI is currently working on the non-thermal plasma applications by way of developing dielectric barrier discharge (DBD) based VUV/UV excimer light sources [1-2] for food and health applications [3].

In the excimer light sources spontaneous radiations that employ non-equilibrium radiation of excimer and exciplex molecules play an important role [4]. The excimers are weakly bound excited states of molecules which do not have a stable ground state. The main advantage of excimer light sources is that they provide high-intensity narrow-band molecular radiation in the absence of a strong molecular bond in the ground state which eliminates radiation absorption in the plasma. There are many methods to generate excimers, such as, corona, high-energy electron beam, X-ray, protons, heavy ions, synchrotron radiation, microwave discharges, etc. However, the DBD based plasmas provide one of the most efficient ways to produce the necessary precursors for excimer formation due to its ability to produce high energetic electrons at high working pressures (≥ 200 mbar). High pressure further promotes the suitable conditions for excimer formation by three-body reactions in the plasma. The excimer formation in the DBD is well favored by high collision rates at elevated pressure and efficient excitation or ionization of precursor species. A review of the plasma chemistry required for the VUV/UV excimer formation along with its current trend in the biological applications (including food and health) will be presented.

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IL-25

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Abstract Awaited

IL-26

Myths of Identifying Long Non-coding RNAs using Whole Exome Sequencing: Challenges and Perspectives

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Abstract

Functional genomics of non-coding RNAs (ncRNAs) have opened a new possibility in identifying cause for diseases with substantial interest in analyzing regulatory effects of genome variation. Characterizing them have also allowed us in improvement of next generation sequencing (NGS) tools and studies on the functional characterization have resulted in data on interactions with their RNA peers, DNA or proteins. With transcriptome and high-throughput sequencing analysis revealing a large number of ncRNAs in various organisms, their role as regulatory elements especially in understanding the function of diseases is of immense value to the research community. That said, so far whole genome sequencing has been used to decipher the pathogenic mutations coming from the exonic/coding part of the genome, With recent studies on identification of non-coding RNAs that tend to have a coding potential and discovery of long non-coding RNAs (lncRNA) from exome sequencing, a crucial challenge to explore the myth remains elucidated: To code or not code for non-coding RNAs is the question, but whether or not this emergence of lncRNAs have a role to play with their interaction with its peers for a disease phenotype remains to be answered. We discuss the role of lncRNAs, specific to our phenotype of interest, *viz.* Congenital Pouch Colon (CPC), a rare genetic anamoly.

Keywords: non-coding RNAs, transcription, regulation, genome organization, biomarkers, variation, functional genomics

IL-27

Synthesis of Polyheterocyclic Compounds *via* Transition Metal Catalyzed C-H Functionalization

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Formation of carbon-carbon (C-C)/carbon-heteroatom (C-X) bond through transition metal catalyzed C–H functionalization has attracted much attention in comparison to traditional methods as it avoids pre-functionalization of substrates and provides straightforward access to structurally diverse and complex molecules under eco-benign conditions from simple substrates.[1] Moreover, development of novel synthetic transformations that involve tandem C-C/C-X bond formation processes and complexity generating reactions under the same reaction conditions has become very attractive and highly desirable in organic synthesis. Such processes reduce chemical waste generation and reaction time.

On the other hand, synthesis of polyheterocyclic compounds (PHCs) has attracted significant interest in modern drug discovery (PHCs) because of their varied biologically and interesting pharmacological properties.[2] Our group has been working towards developing reaction methodologies through transition metal catalyzed transformations involving tandem C-C/C-heteroatom bond formation and/or coupling/C–H functionalization reactions that enable to transform simple starting materials into complex PHCs (Figure 1).[3] Details of the developed methodologies will be presented.

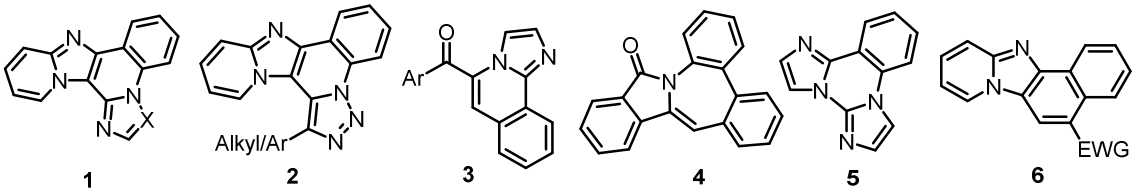

Figure 1: Structure of selected fused aza-heterocycles.

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IL-28

Phosphodiesterase Enzyme: Promising target for Medicinal Chemist

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Abstract:

Cyclic nucleotide phosphodiesterases (PDEs) are enzymes that regulate the cellular levels of the cAMP and cGMP, by controlling their rates of degradation. There are 11 different PDE families, with each family typically having several different isoforms. This isozyme superfamily has now become a major focus of drug discovery efforts owing to its diversity, molecular nature, differential regulation and expression in different cell types, and the range of biological functions. Selective inhibitors for each of the multiple forms of PDE can offer an opportunity for preferred therapeutic intervention and would be an extremely useful target in drug discovery efforts for a medicinal chemist. This thematic issue details many key aspects of multiple forms of PDEs and their inhibitors with diversified chemical structures, which can act as leads for synthesis of novel drugs. In addition, new insights gathered about structure-function relationships will be highlighted, in particular those relating to enzyme regulation.

Keywords: Phosphodiesterases, Phosphodiesterase inhibitors, Medicinal chemistry, and Drug development

IL-29

Transition Metal Catalyzed Dehydrogenative Cross-Coupling: Direct Access to polycyclic Heteroarenes

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Selectivity in organic transformations, be it chemo-, regio- or stereoselectivity is the most challenging to achieve. Chemoselectivity implies the preferential reaction of one functional group over another under the same reaction condition. Regioselectivity is the preferential formation of one isomer of the product over another. The other challenging control is stereoselectivity, where three dimensionally confined molecule synthesis is involved.

C-H activation is emerging as a potential method to achieve complex controlled molecular architectures *via* simple-minimal step strategies. Currently, when progress in C-H activation has overcome the initial barriers related to the low reactivity of the C–H bonds, efforts have been particularly focused on achieving site selective functionalization in the presence of a multitude of C–H bonds by outcompeting the formation of other possible isomers. Moreover, the possibility of intermolecular homo and heterocoupling cannot be overlooked, although they can be avoided through tactful optimization of the reaction conditions. Research efforts for the past few years have made significant progress via the directed group assisted functionalizationfor the regioselective C-H functionalization in arenes and heteroarenes, which interestingly are the most valuable precusers.[1] However, selective distal C-H functionalization in these moieties have not been much explored.In this presentation, a transition metal catalyzed selective distal C-H functionalization of N-substituted pyrrole-azole system will be discussed.[2]As an example of another site-selective C-H activation, a ligand enabled Cu catalyzedintramolecular C-2 site selective Csp^2-H/ Csp^2-H activation method for *N*-substituted pyrrole-azole system will also be presented.[3]Our methodology can be further extended intramolecular C–H coupling reaction between indole-2 and imidazole-2 moieties to deliver annulated polycyclic heteroarenes, via a very simple Cu-salt, which arecomparatively economical and less toxic than other commonly used transition metal salts.[4]

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IL-30

"GREENER" CHEMICAL SYNTHESES FOR BIOINSPIRED METALLO MACROCYCLES: A WINDOW INTO MEDICINAL CHEMISTRY

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ABSTRACT

The varied nature of the chemical world requires various greener pathways in our quest towards attaining sustainability. Green chemistry has come a long way since its birth in 1991, growing from a small grassroots idea into a new approach to scientifically-based environmental protection. The emerging area of green chemistry envisages minimum hazard as the performance criteria while designing new chemical processes. Rather than end-of-the-pipe remediation approach, which involves cleaning up of waste after it has been produced, the main objective is to avoid waste generation in the first place. There are different shades of greener processes being developed as we continue exploring alternatives to conventional chemical synthesis and transformations. The desired approach will require new environmentally benign syntheses. The chemistry of macrocyclic complexes has witnessed an outline by individual scientific backgrounds and individual interest due to their analytical, industrial, agricultural and medicinal. The anticancer properties of square-planner platinum compounds have fueled an interest in the chemistry of all the metal complexes. Keeping all these factors in mind we aimed to synthesize and characterize macrocyclic compounds with N_4 –tetraamide ligands. The main emphasis has been given on in vivo studies on male rats by performing biochemistry and fertility test. The aim is also to prevent the toxic effect or abnormal observations of the pesticides and antifertility agents. Good antimicrobial complexes have been selected for antitumour activity. The positive findings will be discussed in detail.

IL-31

Neuronal Gasotransmitter Delivery with a Redox Trigger

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Soft nanoscale structures present exciting prospect in drug delivery, tissue engineering, and biosensing. It is possible to engineer biocompatibility and stimuli-responsive character, for example pH, ionic strength, temperature, light, and redox environment, in such structures to allow for active molecule encapsulation, followed by targeted delivery. In this talk, I will present two recent approaches for such systems: one involving a photoactivatable dopamine-conjugated platinum anticancer complex incorporated in guanine tetrad-borate hydrogels (1) and the other one consisting of a self-assembling peptide conjugate, carrying a nitric oxide release handle (2).

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IL-32

Catalysis for Green Chemical Production

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Abstract

Catalysis has emerged as a key technology for the sustainable and eco-friendly production of diverse chemicals used today. Around 90% of chemical transformations in industry today use catalysis. The total value of global chemical production depending on catalysis is estimated around US$ 2 trllion. It is further estimated that nearly 20% of the world economy depends directly/ indirectly on catalysis. This is a rare technology which combines both economic and environmental benefits.

This presentation will discuss the increasing influence of catalysis in enhancing the green content in the synthesis of bulk chemicals, polymers, pharmaceutical intermediates and fine chemicals. Presentation will also discuss about the role of catalysis in making availability of renewable feedstock like biomass for future chemical production. Presently, only 5% biocatalysts are commercially used for chemical production. Some of the challenges in the area of developing commercial biocatalysts also be discussed.

IL-33

Cu(II) Complexes of D-glucose derivatives and their application in oxidation reactions

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Carbohydrates are one of the major energy sources for the living beings and they also act as chiral building blocks for the formation of polysaccharides, nucleic acids, and antibiotics. It is widely present in the biological system and controls many life processes in the form of polysaccharides, glycolipids and glycoproteins.Inspired from these facts, we are engaged in developing the organic and inorganic derivatives of D-glucose and studying the chemical as well as biological activities of the synthesized molecules.

Condensation of 4,6-*O*-ethylidene-*β*-D-glucopyranosylamine with salicylaldehyde derivatives affords a series of metal ion chelating ligands. The structure of Cu(II), Ni(II), Zn(II), V(V), Mo(VI) and U(VI) complexes of such ligands has already been established by single crystal X-ray diffraction technique. Among these complexes, Cu(II) complexes are fascinating due to it's variable coordination, 3-D structure and catalytic properties. Simple ligand likeN-(2-hydroxybenzilidene)-4,6-*O*-ethylidene-*β* -D-glucopyranosylamineaffords dinuclear Cu(II) complex,[1] while N-(3-*tert*-butyl-2-hydroxybenzilidene)-4,6-*O*-ethylidene-*β*-D-glucopyranosylamine affords tri- and tetranuclear Cu(II) complexes.[2] In the dinuclear Cu(II) complexes, metal centers are separated by about 3 Å and connected through alkoxy bridge. Catecholase enzyme also possesses an oxo bridged dinuclear Cu(II) system with Cu---Cu distance of about 3 Å.[3] So, we tried our complex as catalyst to oxidize 3,5-di-tert-butylcatachol and succeed in that.[4] After establishing the oxidizing abilities of our complex, we also used these complexes in catalytic oxidation of primary and secondary alcohols.[4] Our compounds selectively oxidizes the primary and secondary alcohols into corresponding carbonyl compounds under mild condition in good to excellent yields.

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IL-34

Waste Biorefinery for Chemical and Fuels

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The impact of waste on environment cannot be neglected and therefore, makes it worthwhile to remediate waste and recover revenues in the form of biobased products. Our research is aimed at overcoming the converging consequences of two issues viz., increasing quantities of waste and the demand for fossil based products. We are working on developing sustainable and advanced waste remediation methods for the production of biofuels and platform chemicals. IICT designed and constructed a state of art pilot plant facility (10,000 liters capacity) for the production of biohydrogen from waste/wastewater with the funding from Ministry of New and Renewable Energy, Government of India. The pilot plant was operated with the food waste at organic load of 55 g COD/l after pre-hydrolysis (12 hours) in a acidic microenvironment using selectively enriched consortia as biocatalyst with 48 hours of retention time. The facility generated biohydrogen of 54,000 l/day with a COD removal efficiency of 44%. A holistic approach for the production of biobased products utilizing waste would be by designing a biorefinery with a closed loop approach. Acid rich effluent generated from acidogenesis is potential feedstock for the production of various biobased products, thus increasing the treatment efficiency by closing the loop in a biorefinery format. In order to effectively utilize the waste, the pilot plant was integrated to a waste biorefinery platform designed and constructed by CSIR-IICT (funded by CSIR, Government of India; 12 FYP- CSC-0113) with operation capacity of 10,000 liters. The biorefinery facility consist of anaerobic reactors (2 no), algal race way ponds (2 no), ecological engineered living system (three stages), PDBR system(anoxic/aerobic) and bio-electrochemical treatment system connected in a defined/sequential order to recover biobased products in a cascading way by passing wastewater in a closed loop from biohydrogen production (for dilution) to organic farming. This communication make an holistic attempt to establish a systematic link between waste remediation and biobased products, accounting for a paradigm shift from ‘waste as pollutant’ to ‘waste as wealth’.

IL-35

HIGH PERFORMANCE POLYMERIC NANO COMPOSITE AND ITS TECHNOLOGICAL APPLICATIONS

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Abstract: The present investigation highlights development of high performance polymeric nano composite based on polyether ether ketone (PEEK) (service temperature – 250^{0}C to +300^{0}C, tensile strength: 120 MPa) and ultra-high temperature resistant epoxy adhesive (DURALCO 4703, service temperature -260^{0}C to +350^{0}C and its fabrication by high performance nano adhesive for its essential application to aviation, automobile and aerospace industries. High performance nano adhesive is prepared by dispersing and carbon nanofibre into ultra-high temperature resistant epoxy adhesive. The surface of PEEKis modified by low pressure plasma and atmospheric pressure plasma, prior to bonding. It is observed that polar component of surface energy leading to total surface energy of the PEEK increases significantly when exposed to atmospheric pressure plasma. The fractured surface of the adhesively bonded PEEK is examined under SEM. It is observed that unmodified PEEK fails essentially from the adhesive to PEEK interface resulting in low adhesive bond strength. Electron Spectroscopy for Chemical Analysis (ESCA) reveals that the polymer surface becomes hydrophilic resulting in increase in surface energy. Thermo-Gravimetric Analysis (TGA) studies show cohesive properties of nano adhesive is more stable when heated up to 350^{0}C. Adhesive joint strength of surface modified PEEK increases considerably and there is a further significant increase in bond strength when it is prepared by carbonnanofibre epoxy adhesive.PEEK is being used for biomedical applications because it has good biocompatibility, high mechanical properties, chemically stable and its elastic modulus is nearer to that of normal human bone.

Key Words: Poleyetherether ketone (PEEK), epoxy adhesive (DURALCO 4703), Low Pressure Plasma, Atmospheric Pressure Plasma, carbon nano fiber, Adhesive Bond Strength.

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IL-36

Waste Biorefinery for Chemical and Fuels

Anshu Dandia

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Abstract Awaited

IL-37

Chemistry of carbon dioxide: Greener applications & synthetic explorations

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Abstract:

The production of carbon dioxide around the globe resulting the emergence of global warming day by day. Burning of coal, vehicles fuel, natural gas and nuclear explosions also generates carbon dioxide in the environment, has been the major constituents which majorly influences the global warming. This burden of carbon dioxide in our environment necessitates the need of transforming carbon dioxide into greener valuable products. Also, carbon dioxide has been playing an important role in balancing our environment through photosynthesis in plants.

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 recent years, chemistry of carbon dioxide has been explored in many ways starting from the renewable source of energy to the synthesis of biologically potent scaffolds. In the present talk, I will focus some of the greener applications of carbon dioxide as a source of renewable energy along with many synthetic explorations.

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IL-38

Correlating Morphology and bonding environment in freestanding thin films

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Abstract

Free-standing flexible thin films of polymers- pristine as well as doped were prepared with PVDF as the host matrix and inorganic dopants using sol-gel technique. These films for a class of Organic Semiconductor Inorganic Dopants (OSID) thin films useful in modern generation device applications. The films were characterized for morphological and bonding environmental modulation due to various factors- dopants, electrical poling,etc. A Carl Zeiss AURIGA FIB/FESEM system was used to record the surface morphology. To understand the bonding environment, X-ray Photoelectron Spectroscopy (XPS) measurements and Raman studies were carried out. Distinct variation in the texture due to poling could be observed. The texture of the un-poled PVDF film is smoother and depicted fibrous features while the poled samples showed a rougher surface for either side of the film surface. This could be correlated with the terminal elements in the chemical structure of the PVDF. The difference in the ionic radii of the terminal elements would result in such variations. The centro-symmetry of the dopants when introduced in the PVDF matrix appears disrupted. This article discusses the variation in the morphology and attempts to provide a possible explanation with the modulation of the bonding environment.

IL-39

Air Quality Studies to Address Uncharted Sources of urban climate in India

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Abstract

Air pollution, reported to claim 25 lacs lives every year in India, is mainly occur due to emissions resulting from several anthropogenic sources in urban environments of India; including industrial activities, road-traffic, household solid fuel use and construction activities. Current challenges to address the air quality of urban environment including assessments of air pollution levels in classified atmospheric receptors, sources of air pollution mass and impacts in human health required to define the objectives, study design, sampling plan, selection of air samplers and instruments for characterization of pollution mass. This presentation describes the various objectives, currently in use, to address the air quality, air samplers to measure aerosol fractions, and findings of selected studies, conducted in recent years.

IL-40

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Abstract Awaited

IL-41

USE OF METALS & MINERALS AS MEDICINE AND CONCEPT OF SHODHANA & MARANA: A NEW PHARMA CONCEPT

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ABSTRACT

Ayurveda is a holistic medical science which is dedicated to mankind. Earlier herbs were more prevalent in treatment and later Minerals & Metals were included for prevention and prolongation of life. Thus, Rasachikitsa (Herbo-Mineral & Metal therapy) came into existence with complete description of minerals & metals along with their processing and therapeutic utility.

But, Since past few decades the age old Ayurvedic heritage is taking many ups and downs because of several reasons. Particularly the Mineral/Metal compounds are being targeted repeatedly by so called western scientists which is letting down the reputation of the Age old Ayurveda.

The Vijaya times in its 20-12-2004 commented “Ayurvedic drugs are questioned for containing dangerous levels of Pb, Hg, As” following a study of the Harvard Medical School. Again similar report was found in the issue of JAMA 14 to 70 different Ayurvedic drugs brought from South Asian Grocery of the Boston area in US have potentially harmful levels of Pb, Hg, As etc.. Later both the authors mentioned that due to ignorance of Pharmaceutical process of Ayurveda the report was made.

Hence, the present paper highlights during the seminar about the various traditional pharmaceutical processes and how these converts toxic metallic- mineral drugs into non nontoxic (safe) medicaments etc...

IL-42

Surface modification of metal oxides by dopant containing organic compounds and application in surface doping of silicon nano-structure

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Surface functionalized metal oxide nanoparticles are widely used in the context of sensing, catalysis, chromatography *etc*. Several reports demonstrate the introduction of organo-boron or organo-phosphorus surface functionalities *via* molecular linking groups, where the organic linker group is reacted to form a covalent bond at the nanoparticle surface and the boron or phosphorus moiety is hanging at the surface. The doping of semiconductors in controlled manner is challenging in the context of modern device architectures. Sharp junctions and localized dopant concentration are important to fine-tune the electronic structure and nano-scale properties. Controlled surface doping may play an important role in doping current semiconductor devices for practical nano-wire based devices and photovoltaic building blocks. Conventional doping methods such as ion implantation or solid-source diffusion for controlled nanometer scale surface doping is challenging due to limitations such as nano-scale lattice damage, dopant equilibration throughout the nanostructure *etc*. In the context of semiconducting NW's the commonly used *in situ* CVD doping method suffers from several limitations, including non-homogenous dopant distribution resulting from continuous exposure of the growing SiNW to the dopant precursor, such as phosphine, along the CVD process. A new doping method for the controlled surface doping of silicon wafers and nanometer scale structures is developed. The method, monolayer contact doping (MLCD), utilizes the formation of organo-phosphorus and organo-boron monolayer on a donor substrate that is brought to contact and annealed with the interface or structure intended for doping. A distinctive feature of the MLCD process is that the monolayer used for doping is formed on a separate substrate which is distinct from the interface intended for doping. Organo-phosphorus compounds like triphenyl phosphine oxide which has P=O functional group and organo-boron compound like dichlorophenylborane were used as dopant source.

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IL-43

Glutaraldehyde as suitable substrates for aminocatalytic annulation reactions: Synthesis of medium sized *N*-heterocyclic compounds

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Organocatalysis has grown-up rapidly and applied successfully to several different enantioselective reactions in last one decade and therefore, now considered as the "*third pillar*" of enantioselective catalysis, together with biocatalysis and metal catalysis.[1] Additionally, nitrogen heterocycles constitutes a number of small molecule natural products (SMNPs) acts as therapeutic agents for the treatment of a plethora of diseases that confront humankind in an age where the rapid emergence of multi-drug resistant forms are becoming an increasing threat. In the continuation of our interests,[2] recently we have developed new methods for the asymmetric and non-asymmetric synthesis of medium sized nitrogen heterocycles targeting SMNPs using aminocatalyzed transformation of dicarbonyls through donor-acceptor (D-A) annulation approaches. Details of the D-A concept, design and synthetic strategy for medium sized nitrogen heterocycles using glutaraldehyde will be presented here.

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IL-44

Green chemistry concepts and its role for sustainability towards the development of Multi-component reactions

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Abstract

In all over the globe, Green chemistry concepts and its role are great challenges towards the development of biologically and pharmacologically active heterocyclic scaffolds via multi component reactions. These concepts clearly describes new carbon-carbon and carbon- nitrogen bond formations in such name reactions with using important catalyst which are very selective, simple, ecofriendly, high yielding, and describe concepts tailored to generate substances quickly by joining small unites together. The various products obtained from the different name reactions likewise: knoevenagel condensation, Mannich, Hantzsch and Beginelli are the important class of target molecules due to their biological and biological importance. We were encouraged to combine different Heterocyclic moieties with hydroxyl derivatives of phenol, urea/thiourea, semicarbazide, primary/secondary amines, different 1,3-diones, ammonium acetate, malononitrile, ethyl-2-cyanoacetate and cyanoacetamide in a single molecular framework. In addition to this, we have synthesized a library of thiophene, quinoline and indole incorporated highly functionalized molecules *via* green chemistry approach. All the diversely functionalized molecules were synthesized from commercially available starting materials in one-step reaction gives very good yield using different catalyst. The obtained products were screened for antitubercular, antimicrobial, and cytotoxic activities and some of the single crystals studies were to be discussed.

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IL-45

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Abstract Awaited

IL-46

New Triterpenoid from the Aerial Part of *Phlebophyllum kunthianum*

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In the last few years, there has been an exponential growth in the field of development of drug from plants and gaining popularity both in developing and developed countries because of their natural origin and less side effects. Some of these plants contain substances that can either be directly used as drugs for therapeutic purposes and or may be precursors/ lead molecules for the synthesis of semisynthetic drugs.Medicinal plants continue to be an important source of new therapeutic aid for alleviating ailments of humankind. Keeping in view importance of medicinal plants in therapeutic area and continuous of our ongoing programme/effort to search the novel active/ inactive plants constituents [1,2], recently we have isolated and identified the new triterpenoid from the ethanolic extract of the aerial part of *Phlebophyllum kunthianum*.The details isolation procedure, structural elucidation of the isolated triterpenoid will be discussed during presentation.

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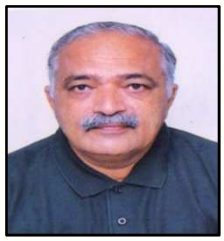
IL-47

Fluorine Chemistry–An important tool for new drug discovery program in the 21st century



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Abstract

A cursory inspection of the medicinal chemistry literature reveals two obvious themes in the structures of current drug candidates: the ubiquity of nitrogen heterocycles and the popularity of organo-fluorine moieties. Therefore, it seems natural that a combination of these two structures will offer rich possibilities in the future of drug development. Fluorine is now present in 20 to 30 % of the drugs of the market. The modulations induced by the introduction of fluorine atoms onto a molecule has a major influence on its behavior within the biological medium such as improvement of metabolic stability, modification of physico-chemical properties such as acidity or basicity of neighboring functions thus acting upon pharmacokinetic properties and direct or indirect impact in interactions between fluorine and proteins [1-3].

Currently more than one fifty fluorinated compounds are used as pharmaceuticals. Therefore, the synthesis of fluorinated molecules play an important role in drug discovery and many pharmaceuticals, a fewwell-knownshining examples are 5-fluorouracil, gemcitabine and emtricitabine,ciprofloxacin, ofloxacin, or norfloxacin, fluconazole, linezolid and tesetaxelpossessed fluorine atoms [4,5].Moreover, fluorine containing heterocyclic scaffolds display quite a broad spectrum of biological activities such as antibacterial [6-8], anti HIV [9], antitumor [10], anti-infective [11], antimalarial [12]and anticonvulsant [13]. In this context, we have synthesized several novel hybrid bioactive motifs clubbed with two or more fluorine containing heterocycles such as pyrazole, quinoline, quinazolinone, thiazole, thiazolidinone, 1,3,4-oxadiazole, pyrimidine and pyridine and these compounds were screened for their antimicrobial activity on several bacterial and fungal strains.

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IL-48

Functionalized Heterocycles as Biologically activePharmacophores and Organic Materials

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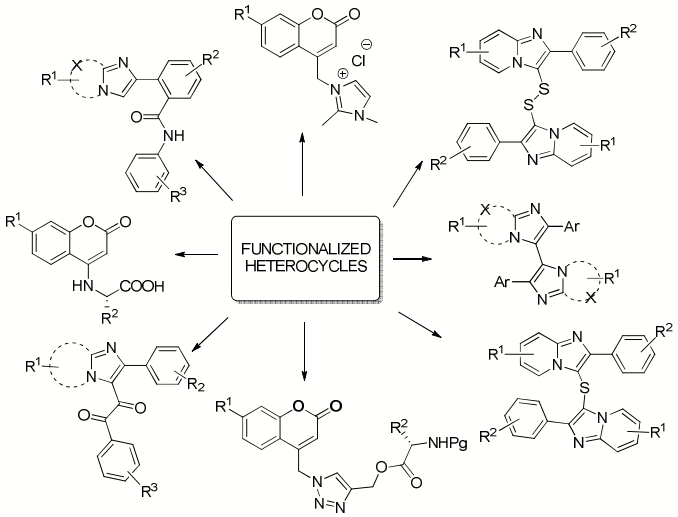
Although numerous advances have been made towards developing metal-free and metal-catalyzed pathways in the domain of functionalization of heterocycles in the past few decades, yet new strategies to exploit their potential as synthetic intermediates to construct biologically important heterocycles, and organic materials continue to emerge. Apart from conventional condensation and coupling methodologies, metal-free and metal-catalyzedcycloaddition, cross-coupling and C-H activation strategiesremain powerful tools for the construction of diverse array of functionalized heterocycles possessing varied applications in medicinal and material chemistry. In regard to these aspects, some recent results[2] on the development functionalized heterocycles, and their applications (Figure 1) will be discussed.



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ISCB AWARDS

ISCB Pof. Jyoti Chatterji Prize for Excellence-2018

NMR studies of G-rich DNA fragments that fold into G- and AGCGA-quadruplexes

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Double stranded helix is the most common secondary structure of DNA. When DNA is involved in processes such as replication and transcription, its double helical structure is partially unwound into two strands. Switching to single strands under certain conditions leads to formation of higher-order DNA structures which can interfere or even stop replication possibly resulting in harmful mutations. Guanine- and cytosine-rich sequences may fold into tetrahelicalstructures called G-quadruplexes and i-motifs undercertain conditions, respectively. G-quadruplexesare noncanonical fourstrandedstructures consisting of stacks of guanine residuesassembled into G-quartets and coordinated with intercalated cations such as potassium and sodium. These structures exist in dynamic equilibriumwithin the single-stranded G-rich DNA generatedduring major genomic events (replication, transcription).G-quadruplexesmay be modulators of nucleic-acid-processingproteins and, as such, as potential components of newpathways of genome and epigenome regulation.Solution-state NMR spectroscopy has contributedsignificantinsights that helped to uncover overall topologies and local features of non-B-DNA structural families alone or in interaction with other molecules such as small molecule ligands. An unexpected four-stranded structures stabilized by G-A and G-C base pairs stimulated us to explore if G- and A-rich repeat segments of DNA can adopt tetrahelical structures different from G-quadruplexes. 5'-AGCGA-3' repeat sequences are found in regulatory regions of 38 different human genes linkedto neurodevelopment and neurological disorders, abnormal cartilage and bone formations, cancer and regulation of basic cellular processes. In contrast to the expected G-quartet-based topologies adopted by 5'-GGG-3' repeats structures are stabilized by G-C, G-A and G-G base pairs that interact to form unique structures. In comparison to G-quadruplexes novel structural family does not show the same sensitivity to the presence of cations. New structures suggest that folding landscapes and structural diversity of DNA oligonucleotides are much more complex than previously assumed.

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ISCB Excellence Award 2018

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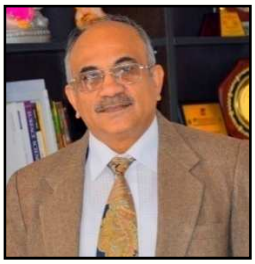

Abstract Awaited

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Rajneesh Mishra

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Abstract Awaited

ISCB Young Scientist Award 2018

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Abstract Awaited

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Vinita Chaturvedi

Senior Principal Scientist, Biochemistry Division, Central Drug Research Institute, Lucknow, India

Abstract Awaited

ISCB Best Teacher Award 2018

Mahesh C. Sharma

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Abstract Awaited

ISCB Best Thesis Award 2018

Dharmendra Singh

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Abstract Awaited

ORAL

O-1

DESIGN AND SYNTHESIS OF FUNCTIONALIZED ORGANIC-INORGANIC HYBRID NANOMATERIALS AND ITS APPLICATION IN ENVIRONMENTALLY BENIGN REACTIONS

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At present, one of the major concerns of the global vision of world economy is the ability to meet the challenges of energy and sustainability. Catalysis can assist in meeting those challenges through the development of greener synthetic routes to address ecological and environmental concerns. In recent years, substantial progress has been made to explore novel approaches for the fabrication of organic-inorganic hybrid nanostructures that offers excellent prospects in designing highly selective and versatile catalytic systems. Recently, heterogenization of active catalytic species has emerged as an elegant and ingenious methodology to generate catalytic materials that possess immense potential to accelerate chemical transformations with enhanced selectivity, excellent durability and recyclability. In this perspective, silica nanospheres have captivated the interest of scientific community as exceptional support matrices since they display numerous unique physiochemical properties such as high surface area, good accessibility, and nanometre size, excellent thermal and mechanical stability. Within this framework, the development of silica based functionalized organic-inorganic hybrid nanomaterials and their structure has been studied using several characterization tools such as TEM, SEM, XRD, FT-IR, BET and elemental analysis. Subsequently, the catalytic efficacy of these nanostructures has been explored in degradation of highly toxic persistant pesticides that do not break down easily or break down very slowly and remain in the environment after a growing season. The utilization of synthetic pesticides has become an essential requirement in agriculture for the control of pests. Pesticide use raises a number of environmental concerns. Organohalide and organophosphorus pesticides remain prevalent in the environment and safe methods for their degradation are needed. Most of the pesticides are resistant to biodegradation and are found to be carcinogenic in nature even at trace levels. Therefore, it becomes essential to develop new technologies which are capable of removing pesticides even at trace levels. Overall, The design and synthesis of functionalized organic-inorganic hybrid nanomaterials and the conversion of hazardous pesticides into less toxic chemicals by using these efficient hybrid nanomaterials will be presented as this is one of the most promising and sustainable route to solve the environmental crisis.

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O-2

"Sultam" and "Sultone" chemistry in Modern Research

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Sulfonamide (SO_2NH_2) and sulfonate (SO_2O^-) are the key groups of several important drugs and likewise sultams (cyclic sulfonamides) and sultones (cyclic sulfonates) manifest a wide spectrum of bioactivities, such as antiviral, antimicrobial, antileukemic, anticancer, enzyme inhibition, etc.[1,2] The presentation will be highlighted on the two main sections of sultam and sultone chemistry through some recent examples.[3-8] The first part will focuses on the recent development of powerful synthetic methodologies related to different transition metal catalyzed cyclization reactions and other different metal-free systems for the synthesis of sultams and sultones. The second part will be highlighted on the recent synthetic applications of sultams and sultones in the synthesis of heterocycles, drug-like molecules and natural products and also recent biological applications of sultams and sultones. In particular, the discussion will be surrounds on the recent developments of different fused-sultams and fused-sultones, precisely talking about the benzosultams and benzosultones from our group. The details will be presented in the conference.

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O-3

Chromium in Environment, Its Toxic Effect from Chromite Mining and Ferrochrome Industry: South Africa

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Abstract: The global demand for chromite ($FeO.Cr_2O_3$), is driven by the need for ferrochrome used in manufacturing different materials[1]. The chromite mining as well as the overall mining sector in South Africa has historically been a crucial factor in the economic growth and advancement of the country [2]. The sector has contributed to the development of an extensive and efficient infrastructure and has led to the establishment of secondary industries [3].South Africa (SA) holds 72 to 80 per cent of the world's viable chromite ore reserves. The country is also the world's largest single producer of ferrochrome and supplies much of the world's stainless steel producers and thus the growing market for their product.Ferrochrome is manufactured in ferrochrome foundries using electric arc furnaces. The ferrochrome process create two different waste products, slag and dust, which both can contain large amounts of Cr(VI) dependent on the process used [4]. The slag portion of the waste makes up the largest volume and is typically discharged into dump sites [5]. Natural leaching and exposure of these dumps can lead to the remobilization of Cr(VI), which pose a major environmental concern [6].The release of Cr(VI) into the surrounding environment can lead to bioaccumulation in humans and mammals, while also causing major health issues [7].

Chromium, in its trivalent state, readily precipitates as chromium hydroxide, $Cr(OH)_3(s)$, at near neutral to alkaline pH conditions (pH > 6). The tendency of Cr(III) to precipitate makes Cr(III) less mobile in the environment and therefore much easier to manage its ecological impacts than for Cr(VI) [8,9]. On the other hand, the hexavalent form of chromium is highly mobile in water and is known to be carcinogenic in mammalian cells [10,11].The objective of this study is to look chromium pollution due to chromite mining and ferrochrome industry in South Africa and its impact on environmemt.

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O-4

Rational design, synthesis and antimicrobial properties of thiophene derivatives that inhibit bacterial histidine kinases

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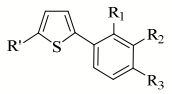
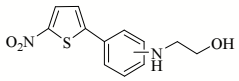
The emergence of multi-drug-resistant bacteria emphasizes the urgent need for novel antibacterial compounds targeting unique cellular processes. Two-component signal transduction systems (TCSs) are commonly used by bacteria to couple environmental stimuli to adaptive responses, are absent in mammals, and are embedded in various pathogenic pathways.[1-6]

To attenuate these signaling pathways, we aimed to target the TCS signal transducer histidine kinase (HK) by focusing on their highly conserved adenosine triphosphate (ATP)-binding domain.[7,8] We used a structure-based drug design strategy that begins from an inhibitor-bound crystal structure and includes a significant number of structurally simplifiying “intuitive” modifications to arrive at the simple achiral, biaryl target structures. Thus, ligands were designed, leading to a series of thiophene derivatives. These compounds were synthesized and evaluated in vitro against bacterial HKs (Figure1). We identified eight compounds with significant inhibitory activities against these proteins, two of which exhibited broad-spectrum antimicrobial activity. The compounds were also evaluated as adjuvants for the treatment ofresistant bacteria. One compound was found to restore the sensivity of these bacteria to the respective antibiotics.[9]



6a: R'=NO_2, R_1=NH_2, R_2=H, R_3= H
6b: R'=NO_2, R_1= H, R_2=NH_2, R_3= H
6c: R'=NO_2, R_1= H, R_2=H, R_3= NH_2
6d: R'=NO_2, R_1=OH, R_2=H, R_3= H
6e: R'=NO_2, R_1= H, R_2=OH, R_3= H
6f: R'=NO_2, R_1= H, R_2=H, R_3= OH
6g: R'=CH_3CO, R_1=NH_2, R_2=H, R_3= H
6h: R'=CH_3CO, R_1= H, R_2=NH_2, R_3= H
6i: R'=CH_3CO, R_1= H, R_2=H, R_3= NH_2
6j: R'=CH_3CO, R_1=OH, R_2=H, R_3= H
6k: R'=CH_3CO, R_1= H, R_2=OH, R_3= H
6l: R'=CH_3CO, R_1= H, R_2=H, R_3= OH
6m: R'=$NHCOCH_3$, R_1=NH_2, R_2=H, R_3= H
6n: R'=$NHCOCH_3$, R_1= H, R_2=NH_2, R_3= H
6o: R'=$NHCOCH_3$, R_1= H, R_2=H, R_3= NH_2
6p: R'=$NHCOCH_3$, R_1=OH, R_2=H, R_3= H
6q: R'=$NHCOCH_3$, R_1= H, R_2=OH, R_3= H
6r: R'=$NHCOCH_3$, R_1= H, R_2=H, R_3= OH
6s: R'=NO_2, R_1=OCH_3, R_2=OCH_3, R_3= H
6t: R'=CH_3CO, R_1=OCH_3, R_2=OCH_3, R_3= H
6u: R'=$NHCOCH_3$, R_1=OCH_3, R_2=OCH_3, R_3= H



7a (ortho position)
7b (meta position)
7c (para position)

Figure 1.Chemical library designed, synthesized and biologically evaluated

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O-5

MULTISTAGE INHIBITORS OF MALARIA PARASITE VITAL FOR MALARIA ERADICATION

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Despite the several major scientific and technological advances, malaria causes millions of deaths yearly, particularly in the endemic regions. The failure of current therapeutics and paucity of new efficient drugs together create the additional burden to the global public health. Indeed, it is hard to name a single effective drug that does not face the resistance to the parasite. Unfortunately, majority of the frontline malarial treatments target blood stage of the parasite. Renewed malaria eradication guidelines advise the discovery of new drugs that target liver, asexual, and sexual blood stages (that is, multistage activity) with clear mode of actions. Considering these facts, we developed a chemical library based on synergistic association of high-valued heterocycles with phthalimide and hydroxyethylamine scaffolds. The biochemical assays suggested few potential molecules that exhibited significant growth inhibition of *Plasmodium falciparum* in culture and *Plasmodium berghei* infection in mouse model with minimal cytotoxicity. Selected hits were evaluated as noteworthy multistage growth inhibitors (liver, asexual blood and gametocyte stages) of the parasite in low micromolar inhibitory concentrations. Structure-activity relationship indicated the vital role of amino acid linkers for obtaining the maximal antimalarial activity. Additional experiments displayed synergistic interactions with chloroquine and dihydroartemisinin in culture and *P. berghei* infected mice model. Few hits were investigated for their target deification and found to inhibit the activity of plasmepsin (II, IV and V), enzymes found in the digestive vacuole of the plasmodium parasite. Plasmepsin V has been recently investigated as a crucial for parasite life cycle and hence represent a potent drug target. Overall, we present a new class of chemical compounds that are capable to intervene the multiple life stages of the malaria parasite inhibitors that could be of great value to direct the progress of drug discovery in the area.

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O-6

Developability Assessment of an IgG2 Monoclonal Antibody Prior to Commencement of Process Development

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Monoclonal antibodies (mAbs) have become the predominant category of protein-based therapeutic agents. Although IgG monoclonal antibodies have highest success rate than other therapeutic proteins, projects terminated due to structural variability are common. Developability studies have therefore become significantly important to select leading candidate molecules for development. Candidates that have potential issues will be eliminated at early stages or redesigned to avoid future risk during the development and manufacturing.

Here an oxidation study on an IgG2 molecule will be presented. Through applying specific set of stress conditions and analyzing the stressed samples using ion exchange chromatography, subunit and peptide map LC-MS, the oxidation pathway of this IgG2 mAb was revealed. As oxidation can occur during up- and downstream process, formulation and storage, and has a potential of affecting mAb structural stability, biological activity and immunogenicity, evaluating oxidation potential and pathway serves as an integral part of forced degradation study to access developability.

O-7

Reduce energy consumption and greenhouse gases emitting in the distillation unit using the feed- product heat exchanger

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Abstract

It is generally accepted that greenhouse gas emissions leads to global warming. About 75% of the anthropogenic emissions of carbon dioxide come from the combustion of fossil fuels. The biggest refinery plant in Northern East of Iran is Khangiran sour gas refinery plant. This refinery have two distillation unit with one distillation tower in each units. This units are the same as each other and produce solvent cut, naphtha cut, kerosene cut and bottom diesel cut. The feed tray location is sixth tray with feed rate about 4.125 tons per hour and feed temperature about 40 °C . The diesel cut is sent to the storage tank with the temperature of 100 °C therefore a lot of energy were wasted. In order to reduce fuel consumption in furnace, a heat exchanger was installed to contact feed stream and diesel cut.

This paper examined the effect of heat exchanger installation on furnace fuel consumption and carbon dioxide (CO_2) generation. In this paper heat exchanger was simulated with several heat exchanger configuration. The results show that due to heat exchanger installation, furnace fuel consumption reduces about 116.21 SCM per day . Also, it was shown that the preheating strategy was suitable from environmental viewpoint and caused reduction of 75.822 metric ton of CO_2 emission per year. Furthermore statistical results show that while a heat exchanger be used furnace performance becomes better.. Moreover, the results show that furnace efficiency increased, while an inlet temperature was increased.

Key words: greenhouse gases, distillation unit, preheating strategy

O-8

COMPUTER AIDED DRUG REPOSITIONING AND BIOLOGICAL EVALUATION AGAINST PARKINSON DISEASE

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Abstract :-

`Parkinson disease (PD) is a common, slowly progressive neurodegenerative disease. The clinical manifestation of PD occurs when about 50 percent of nigral dopaminergic neurons and 70 percent of straital dopamine fibres are lost. The present work was aimed at discovering anti-parkinson potential of existing old drugs using *in silico* repositioning tools. Ligand and structure based *in silico* methods were employing end screen the potential candidates against known anti-parkinson's query molecules. In the ligand based approaches, established drugs, successfully repositioned drugs and clinical trial candidates from antiparkinson's category were collected from the published literature and used as reference query molecules .In shape based and 2D fingerprinting having score 0.7 were shortlisted. Bayes classification model to predict these selected candidates for anti-parkinson and non-parkinsonian activity.In the structure based approaches moleculer docking has been been acknowledged with significant attention among all the virtual screening methods. Glide energy grids were generated for each the prepared complexes which used for docking and scoring calculation to predict binding affinity. Pharmacological screening of the selected test drugs has been performed both, *invivo* and *invitro*. The test result clearly demonstrated that drugs like sulfasalazine and mesalazine were found more effective among all, in the majority of both drugs showed better activity in most of the behavirol and biochemical studies. The *in silico* techniques have been successfully employed in the present research to identify and reposition some potential candidates against PD. The *in silico* predictions were validated in the laboratory and all the selected four test drugs were found to show promising anti-parkinsonian activity in preclinical investigations using rodent model.

O-9

Design, Synthesis and anticancer activity of Imidazo[1,2-*a*]quinoxaline as Inhibitors of Tubulin Polymerization

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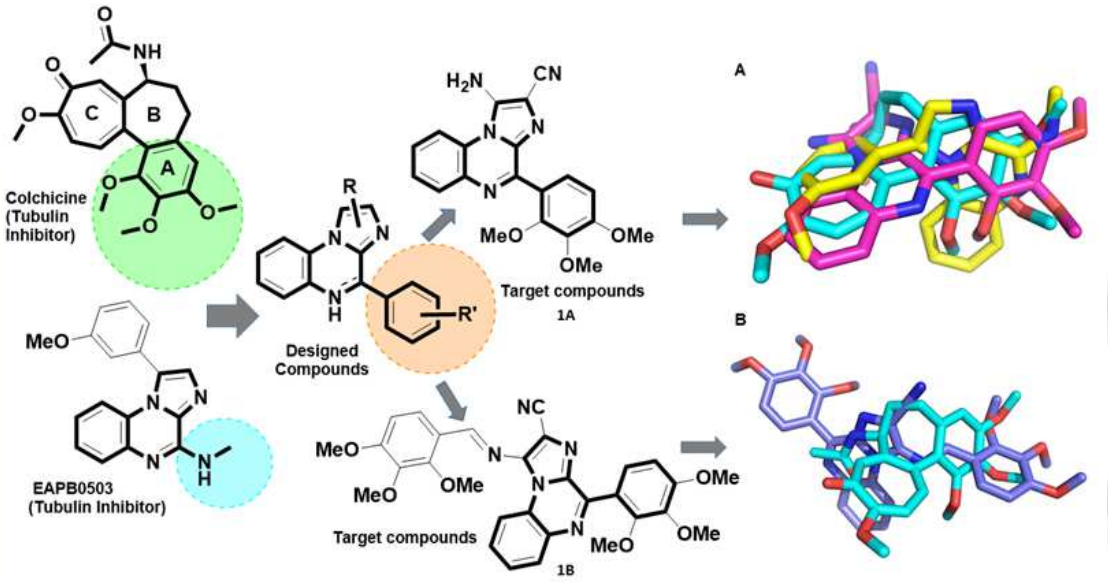
Nitrogen heterocycles are considered as the privileged chemotypes in pharmaceuticals as they constitute about 59% of total US FDA approved small molecules.[1, 2] Among them, imidazoquinoxaline[3, 4] and imidazodiazepine[5] skeletons are widely used in practice due to their broad applications in drug discovery. In particular, imdiazo[1,2-*a*]quinoxaline derivatives possess anticancer (antitubulin; EAPBo503),[6] antiallergic (dazoquinast),[3] anticonvulsant (LU-73068),[7] kinase inhibitory[8] (BMS-345541[9] and AX-13587) activities.

The present work involves the synthesis and biological evaluation of rationally designed antitubulin imdazo[1,2-*a*]quinoxaline[10] derivatives (**1**) having substitution with phenyl ring at -4 position and amino (**1A**) or iminic (**1B**) at -1 and cyano at -2 positions. The designed compounds (**1A** and **1B**) were docked at colchicine binding site of tubulin (PDB: 4O2B)[11] and were found to occupy the cavity where EAPBO503[6] and colchicine bind and possessed all useful residual amino acid interactions and better dock score (Scheme 1). An efficient and straightforward regioselective synthesis of novel imdiazo[1,2-a]quinoxalines was achieved through modified Pictet-Spengler reaction at *C*-2 positionof imidazole of a novel substrate,5-amino-1-(2-aminophenyl)-1*H*-imidazole-4-carbonitrile for the first time, with some carbon electrophiles in high yields. All the compounds were assessed for their anticancer activity and majority of the synthetic molecules were found to possess excellent anticancer[12-14]activity *in vitro*, and mechanistically found to be inhibitors of tubulin polymerization. In addition, synthetics were found to alter intracellular ROS levels, mitochondrial membrane permeability, caused cell cycle arrest and induce apoptosis in the cancer cells.



Scheme 1: Design of imdiazo[1,2-*a*]quinoxaline (1A and 1B) derivatives as tubulin inhibitors

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O-10

Design and Evaluation of Orodispersible Tablets Using Combination of Superdisintegrants

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The oral route remains the perfect route for the administration of therapeutic agents because the low cost of therapy and ease of administration which lead to high levels of patient compliance. Many pharmaceutical dosage forms are administered in the form of pills, granules, powders, and liquids. It is estimated that approximately one-third of the population has pill-swallowing difficulties, primarily the geriatric and pediatric populations. The geriatric and pediatric populations are more prone to have swallowing difficulties. Mouth dissolving tablets having various advantages over conventional solid oral dosage form like swallowing problem especially in geriatric patient and paediatric patients; rapidly dissolve in saliva without the need for water etc. An attempt has been made to design and study of Mouth dissolving tablet of Atenolol by direct compression method. We have done the study of bulk material as well as the properties of designed preparation. Three superdisintegrants (croscarmellose sodium, crospovidone and sodium starch glycolate) were used alone as well as in combination. Fifteen formulations were prepared and all had different concentration level of superdisintegrants to assess their efficiency. Physiochemical properties, in-vitro release characteristics, wetting time and stability profile of optimized formulation were evaluated. Croscarmellose sodium and crospovidone combinations were found to be best among the three alone as well as other combinations of superdisintegrants. Basis of above study can be useful in designing and study of other drugs to develop into advanced dosage forms, which can fulfills emerging demand of population.

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O-11

Sustainable Palladium Catalysis for the Synthesis of Multi-functional Nucleosides in Water

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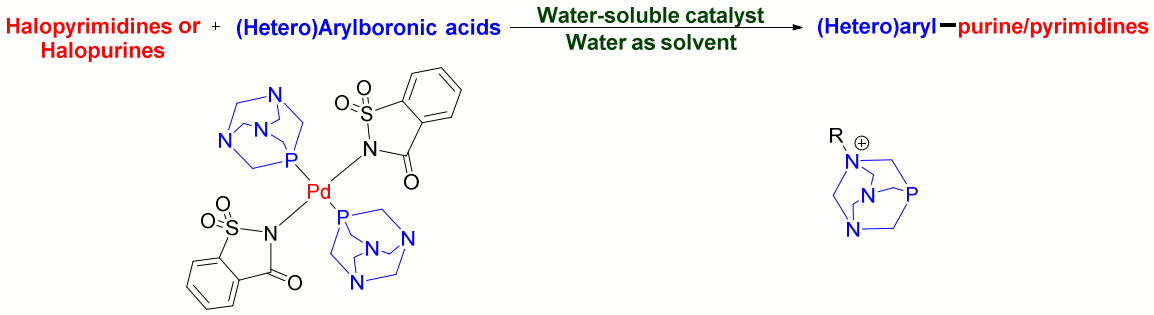
Functionalization of nucleoside heterocycles by transition metal catalysed cross-coupling reactions are important tools to prepare modified nucleoside analogues. Palladium-catalyzed cross-coupling reactions are powerful methods to attach carbon (hetero) atom groups to the heterocyclic base**.** These nucleoside analogues after modification show high fluorescence and biological activity.[1a-e]
The 1st generation palladium complexes allowed the modification of nucleosides in water as the sole reaction solvent for all 4 nucleosides at relatively low catalyst loading.[2]Despite achieving the desired reactivity with the 1st generation catalytic system, column-free isolation of the products or recyclability of the catalyst was not possible. A rational ligand design was therefore needed for the development of 2nd generation Phosphatriazene-based ligands which allowed us to achieve the above objectives.[3]Room temperature modification of nucleosides (new results with 3rd generation) and biological studies (that includes protein sensing) are also included and will be discussed as a part of the presentation.



First Generation Water-Soluble Pd-Imidate **Second Generation Water-Soluble Sultone**

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O-12

BIOSYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL ATIVITY OF SILVER NANOPARTICLES USING LEAF EXTRACT OF *THUJA ORIENTALIS*

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Silver nanoparticles were prepared in a simple, cost-effective and eco-friendly way. Leaf extract of *Thuja orientalis* was used as a reducing and capping agent. The biologically synthesized Ag-nanoparticles were characterized by SEM, TEM, XRT and spectral studies, which revealed that average size of particles, are 18-20 nm. These nanoparticles showed antibacterial activity against E. coli and P. aerogenosa. The problems of environmental pollution may be avoided by this synthetic method.

Key Words: *Thuja orientalis, Biosynthesis, Silver nanoparticles, SEM, TEM and XRT*

O-13

DEVELOPMENT OF IONICALLY CROSS LINKED PHOTORESPONSIVE (TPCC4) CHITOSAN NANOPARTICLE FOR DRUG DELIVERY

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With an objective to improve the photosensitizer efficacy, we have synthesized a tetra-phenyl-chlorin-tetracarboxylate (TPCC4) decorated chitosan nanogel through ionic gelation technique and have investigated its photophysical and morphological properties under different conditions. The TPCC4 based sensitizer, TPCC4 was encapsulated onto the chitosan nanogel, which in turn was prepared through the self-assembly of low molecular weight chitosan (CS) in the presence of sodium tripolyphosphate (TPP) under aqueous conditions. The physico-chemical and photostability properties of the nanogel as well as the photosensitizer loaded nanogel were characterized by employing UV-visible, fluorescence emission, dynamic light scattering (DLS), scanning electron microscopic (SEM) and atomic absorption microscopic (AFM) techniques. The absorption spectra of the free TPCC4 and decorated with chitosan nanogel were found to be similar, whereas in the fluorescence spectra, we observed enhanced fluorescence intensity for the TPCC4 decorated nanogel, when compared to the free TPCC4. The morphological studies through SEM and AFM have indicated that the free nanogel exhibited size in the range *ca.* 80-120 nm with a negative charge of *ca* 1 to -1 mV, while the TPCC4 decorated chitosan nanogel showed *ca.* 100-120 nm. Furthermore, the TPCC4 loaded nanogel showed high photostability, when compared to the free TPCC4 and excellent biocompatibility as evaluated by Alamar Blue reduction assay using human skin fibroblast cell lines. Our results demonstrate that the nano-encapsulation involving hydrophobic interactions significantly enhances the photophysical properties and bioefficacy of the photosensitizer thereby the potential of the nanogel as an effective vehicle for drug molecules and various sensitizers in Photodynamic therapic (PDT) applications.

O-14

Fate of Organochloro and other Pesticide Residues in Soil and Aquatic Environment and their Neuro-toxic Effects

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ABSTRACT

The use of pesticides made possible to a greater extent the prevention of animal and plant diseases and also helped in increased food production. However, pesticides are no found distributed throughout the environment particularly in soil and aquatic environment and cause a number of neurotixic effects as a result of their existence. A general appraisal of the types of pesticides, their pathways into environment as well as the causes for the persistence of pesticides in soil and in aquatic environment as well as the causes for the persistence of pesticides in soil and in aquatic environment are of paramount importance. In developing countries, the environmental impact of these pesticide residues, particularly organochlorines has only slowly become apparent and in many cases the findings caused great concern. Organochloro pesticides normally called as persistent pesticides can get into the body system after bioamplification and further tamper with the mechanism of nerve impulse transmission. In this regard, a thorough understanding of the mechanism of bioamplification mode of physiological action and toxicity and lethal dosage(LD_{50} oral) of pesticide residues is a necessity for an environmentalist in exploring alternatives.

O-15

A general, flexible, ring closing metathesis (RCM) based strategy for accessing the fused furo[3,2-b]furanone moiety present in diverse bioactive natural products

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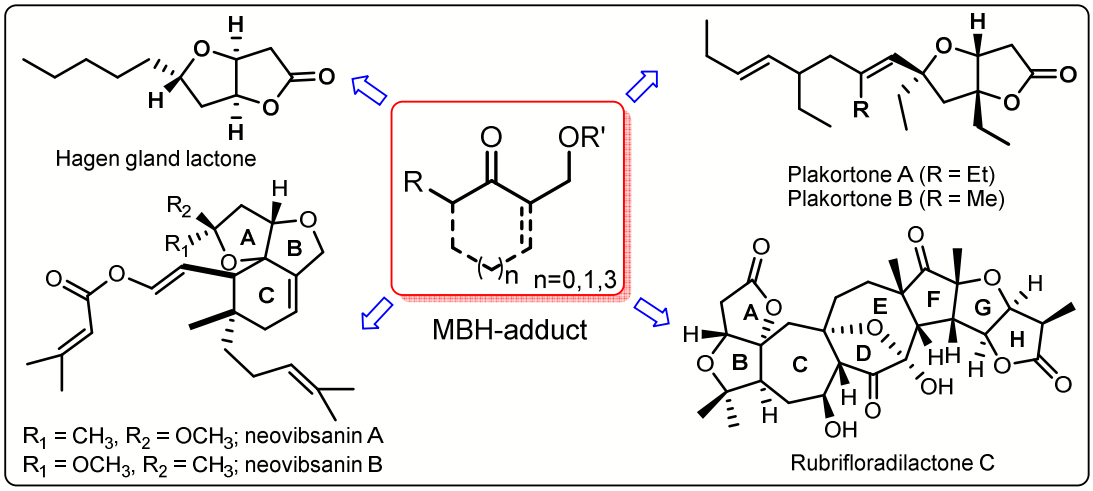
Furo-furanones are the bicyclic compounds in which furan ring is attached to a furanone ring through face-b. Functionally embellished furo[3,2-b]furanone moiety has been widely encountered as a distinctive sub-structure among a diverse range of natural products of mixed biosynthetic origin. Representative examples of natural products incorporating the furo[3,2-b]furanone segment as part of their complex architecture are neovibsanins A and B), lactonamycin, schisandranortriterpenoids (e.g., micrandilactone A), plumericin, pallavicinin and neopallavicinin and plakortones (e.g., plakortone E). A simple and straightforward methodology of general utility to construct sterically encumbered furo[3,2-b]furanone scaffolds present in a diverse range of bioactive natural products is delineated (**Scheme 1**). The methodology emanates from readily available Morita–Baylis–Hillman adducts and employs sequential ring closing metathesis and oxy-Michael addition cascade as the key steps.



Scheme 1. Retrosynthetic analysis for the synthesis of sterically encumbered furo[3,2-b]furanone scaffolds**.**

O-16

Synthesis and characterization of Lanthanide substituted transition metal containing inorganic-organic hybrid polyoxometalates

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Polyoxometalates(POMs) are an important class of metal oxygen anionic nanoclusters with a wide range of structural andchemical properties [1]. Out of the various types of POMs the Keggin type with the molecular formula $[XM_{12}O_{40}]^{n-}$,where the central metal X is generally a p-block element(X= Si^{4+}, P^{5+}, $As^{3+/5+}$) and M is a transition metal in high oxidation state(M= $W^{5+/6+}$, $Mo^{5+/6+}$, $V^{4+/5+}$),is one of the important building blocks for the construction of inorganic-organic hybrids[2]. A few of the oxygen atoms can be removed from the keggin unit to give rise to lacunary POMs. These lacunary POMs behaves as inorganic multi - dentate ligands which are oxygen rich and can easily bind up with transition-metal (TM) or lanthanoid (Ln) cations forming a separate class of POMs known as TM or Ln substituted POMs[3-7]. Our group has reported a number of 3d-4f hybrids based on this type in the recent years.[8-9]

Herein, we have synthesized a series of lanthanide substituted transition metal containing acetate bridged arsenotungstates with the formula $\{[Cu_2(1,10\text{-phen})_2(\mu\text{-}CH_3COO)_2]_4[Ln_2(H_2O)_2(\mu\text{-}CH_3COO)_2(\alpha\text{-}AsW_{11}O_{39})_2]\}^{2-}$[LnIII=Pr(**1a**),Nd(**2a**), Sm(**3a**), Eu(**4a**), Gd(**5a**), Tb(**6a**), Dy(**7a**), Ho(**8a**), Er(**9a**), Tm(**10a**), Yb(**11a**) and Lu(**12a**)].The synthesis involves the reaction of substrates under open air conditions in non-toxic solventsinsteadof the conventional hydrothermal methods. All the compounds were isolated as alkali salts and characterized by single crystal X-ray diffraction followed by FT-IR, UV-Vis spectroscopy, TGA. The single crystal X-ray diffraction analysis for the compounds **(4a)**, **(6a)**, **(7a)**, **(8a)** and **(9a)** reveals that all the compounds are isostructural and crystallizes with Eu**(4a)** in triclinic space group P-1(2) and Tb**(6a)**, Dy**(7a)**, Ho**(8a)** and Er**(9a)** complexes crystallizes in monoclinic system, space group I2/a.

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O-17

Utilizing of *N*-(4)-(benzo[d][1,3]dioxol-5-yl) thiosemicarbazide in the syntheses of various novel types of thiosemicarbazone derivatives: synthesis and antiviral evaluation

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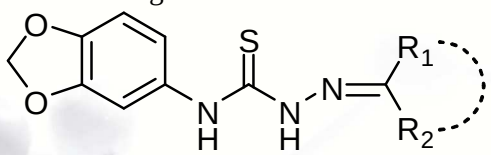
The therapeutic potential of thiosemicarbazone derivatives was first reported in the mid 1940s with *in vitro* assays against Mycobacterium tuberculosis. Owing to their versatile chemistry, research has progressed to the design and synthesis of a broad spectrum of thiosemicarbazone derivatives with antibacterial, antifungal, antiprotozoal and antiviral activities. Thiosemicarbazones possess a wide range of biological activity depending on the parent aldehyde or ketone [1-3].

Large numbers of compounds which contain benzodioxole moiety are known in medicinal chemistry world as important compounds. The SAR information in many publications described that introduction of the methylenedioxy moiety with other moieties led to enhanced biological activity [4, 5].

The aforementioned inhibitory activities of benzo[d][1,3]dioxol-5-yl moiety prompted us to attach benzo[d][1,3]dioxol-5-yl moiety to the thiosemicarbazone. The combination of two privileged structures in one molecule may leads to drug-like molecules. Most of the known thiosemicarbazone derivatives which containing benzodioxole moiety were prepared *via* using benzo[d][1,3]dioxole-5-carbaldehyde for the formation of thiosemicarbazone scaffold block. However, recently, it has been reported that moving a functionalized side chain to the other position can result in retention of biological and providing new opportunities for the design of bioactive compounds. These observations gave us an additional motivation to combination of the thiosemicarbazone scaffold with benzodioxole moiety by using *N*-(4)-(benzo[d][1,3]dioxol-5-yl) thiosemicarbazide. So, novel series of *N*-(4)-substituted thiosemicarbazone derivatives incorporating a benzo[*d*][1,3]dioxole moiety have been synthesized through the reaction of *N*-(4)-(benzo[d][1,3]dioxol-5-yl) thiosemicarbazide with various carbonyl compounds such as aromatic aldehydes, heterocyclic aldehydes, ketones and cyclic ketones. The synthesized derivatives were screened to probe their potential anti-viral activity. The results indicated that the tested thiosemicarbazone derivatives have no antiviral activity or have a toxic effect on the vero cells. Therefore, this study can discovered that incorporation of benzo[d][1,3]dioxol-5-yl moiety into thiosemicarbazone scaffold block is not suitable for a new lead molecule to design more potent anti-viral agents.



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O-18

Natural products based cinnamic acid scaffoldfor novel antifungal drug discovery against *Candida albicans*

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In the last three decades, invasive Candidiasis caused by opportunistic fungal pathogen *Candida albicans* is emerging as severe nosocomial life threatening infections. The eukaryotic nature of fungal cell leaves lesser uniqueness amongst target for drugs making the treatment a primary concern. The development of effective antifungal drugs is lagging behind so much that the existing pipeline has been evidently dry. Due to unavailability of effective drugs, there is an ardent need for suitable alternates and relevant efforts are gradually developing. Natural products have a critical part in antifungal therapeutics for not only being cost effective but rendering lesser toxicity to human host as well. Their gigantic chemical diversity in the structure corresponds to their possibility to interact with myriad of targets. We tested the *insilico*activity of 100 natural product based chemical ligands against major protein targets of fungal pathogen *Candida albicans*. Out of all the compounds tested, the scaffold of cinnamic acid and its derivatives displayed astonishing results. Noteworthy results were observed in 2-coumaric acid, 4- coumaric acid, 3,5-diprenyl-4-coumaric acid, 3-O-prenylcoumaric acid, caffeic acid, and cinnamaldehydebased compounds like 2-nitrocinnamaldehyde and 2-methoxycinnamaldehyde.This work also provides an insight towards *in silico* pharmacokinetic profile of shortlisted compounds with cinnamic acid scaffold. We propose that this study willcontributethe pharmacologically significant natural product based compounds in antifungal drug discovery. While there is still much to be learned with further in vivo models, this study concludes that new ligands can be identified from the existing collection of reference compounds and may it open the gates for identification of new targets in host.

Keywords: Cinnamic acid, *Candida albicans*, Antifungal drugs, Natural compounds, Coumaric acid

O-19

Mono and Dinuclear Cyclic Six-membered Palladium Complexes Derived from Palladium Mediated C-N Coupling of Organonitrile and Formamidine: Synthesis, Structure, Reactivity and Catalytic Activity

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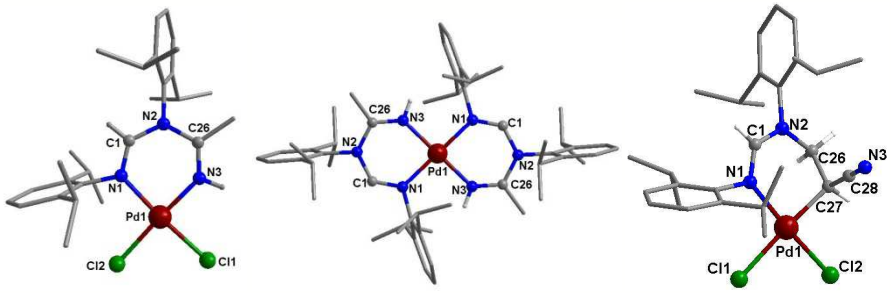
Metal mediated formation of C-N coupled products has been widely studied by taking an organohalide and an amine precursor. There is an alternative method wherein the activated C-N bond of organonitrile can be coupled with a suitable organic precursor [1]. Activation of C-N bond in organonitrile can be achieved by using the nitrile adduct of the metal complexes where in the considerable increase of polarity between C-N will be sufficient to give nitrile-nucleophlic addition, with suitable organic precursors, which cannot be achieved by metal-free synthetic strategies [2]. Following this strategy, reactions of various organonitriles with other nucleophlic reagents led to the formation of C-N, C-O, C-C, C-P and C-S coupled products. Recently, this has been extended to the coupling of the organonitrile and amidine based compounds in the presence of platinum ions [3].During our investigation of the reactions with formamidinium salts and palladium acetate, we have isolated an unprecedented six-membered palladacycle.In this,we discuss the synthesis, structure, reactivity and catalytic applications palladium complexes.Mono and dinuclear palladium complexes are found to catalyze Suzuki-Miyaura coupling of aryl bromides with phenylboronic acid with high yield.



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O-20

MicroRNAs as mediators of viral evasion of the host immune system

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Abstract:

MicroRNAs have emerged as key players in the regulation of various biological processes in eukaryotes, including host-pathogen interactions [1-2]. Recent studies suggest that viruses encode miRNAs to manipulate their host gene expression to ensure their effective proliferation, whereas the host limits virus infection by differentially expressing miRNAs that target essential viral genes (Figure 1) [2-3]. Insect viruses have hardly been the subjects of miRNA investigations. We have identified four *Bombyx mori* nucleopolyhedrosis virus (BmNPV)-encoded miRNAs and also functionally characterized two BmNPV-miRNAs (bmnpv-miR-1 and bmnpv-miR-3) using a combination of *in silico* and experimental methods. Target prediction programme resulted in 8 viral and 64 cellular targets of these virus-encoded miRNAs. We demonstrate the sequence-dependent interaction of bmnpv-miR-1 with Ran mRNA using cell culture and in vivo assays, including RNA interference (RNAi) of Ran. Our results clearly show that bmnpv-miR-1 represses Ran, leading to reduction in the host small-RNA population, and consequently, the BmNPV load increases in the infected larvae. Blocking of bmnpv-miR-1 resulted in higher expression levels of Ran and a decrease in BmNPV proliferation. Whereas, bmnpv-miR-3 is employed by BmNPV, in titrating out its own genes, to avoid host immune response. Our miRNA overexpression and inhibition results showed that bmnpv-miR-3 expresses during early stage of infection, and negatively regulates the expression of DNA binding protein (P6.9) and other late genes. These findings provide an insight into the evasion strategies used by the virus to counter the host defense for its effective proliferation and have relevance to the development of insect virus control strategies.

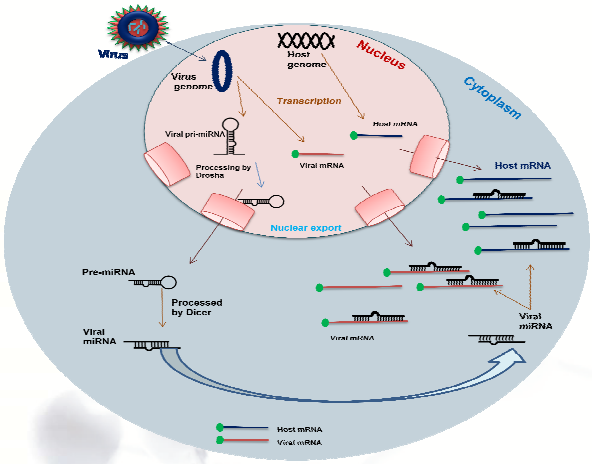

Figure 1: Showing the role of viral-encoded microRNAs in host-viral interactions.

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O-21

[CoIII(L)2]z Complexes (L = Azo-appended *o*-Aminophenol; z = 1–, 0, 1+, 2+). Ligand Redox-Level Mixed-Valency in the Neutral Form

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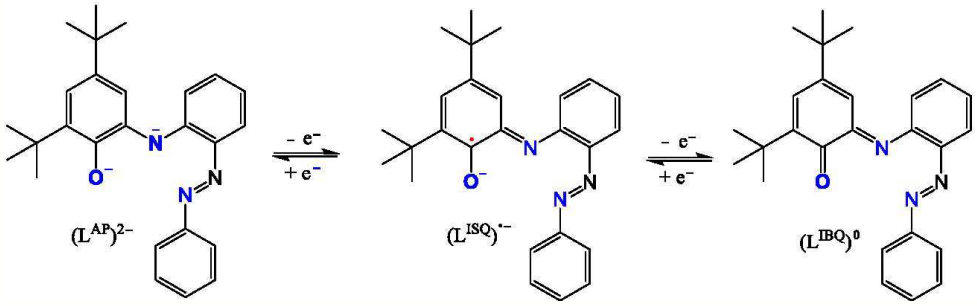

L)2][PF6].2CH2Cl2 (**2**) and one-electron reduction with [CoII(5-C5H5)2] yielded diamagnetic bluish-black crystals (CH2Cl2 solutions display ink-blue color) of [CoIII(5-C5H5)2][Co(L)2].CH3CN (**3**). Coulometric oxidation of CH2Cl2 solutions (containing 0.1 M in TBAP) of **1** at 1.2 V vs SCE produces a light green solution of [**1**]2+ which exhibits an isotropic EPR signal of radical character (g = 2.00). X-ray crystallographic analysis at 100 K points toward [CoIII{(LAP)2–)}{(LISQ}•−], [CoIII{(LISQ)•−}2]1+, and [CoIII{(LAP)2–}2]1– redox-level of the coordinated ligands for **1**, **2**, and **3**, respectively; (LAP)2– and (LISQ)•− represent *o*-amidophenolate(2–) ion and *o*-iminobenzosemiquinonate(1–) radical ion, respectively. The species [**1**]2+ could be [CoIII{(LISQ}•−{(LIBQ}0]2+ (S = 1/2; (LIBQ)0 represents neutral *o*-iminobenzoquinone form of the coordinated ligand). Temperature-dependent magnetism of **1** reveals the presence of a free-radical, which exhibits an isotropic EPR signal (g ~ 2.003) at 298 K and at 77 K an eight-line feature characteristic of hyperfine-interaction of the radical with Co (I = 7/2) nucleus. Thus **1** has an S = 1/2 ground-state. Complexes **1**–**3** and [**1**]2+ species constitute a four-membered electron-transfer series, [Co(L)2]z (z = 1–, 0, 1+, 2+), where only species [**1**]2+ has not been isolated. Spectral analysis justify that the redox processes are ligand-centered, and **1** and [**1**]2+ exhibit localized ligand redox-level mixed-valency. Spectroscopic and redox properties, and Density Functional Theory (DFT) calculations at the CAM-B3LYP-level of theory adequately describe the electronic structure of **1**, [**1**]1+, and [**1**]1–. The observed UV−vis−NIR absorptions for **1**, **2**, and **3** have been assigned, based on time-dependent (TD)-DFT calculations.

O-22

SYNTHESIS AND EVALUATION OF ANTIVIRAL ACTIVITY OF SOME NOVEL HYDROXYBENZYLIDENE THIOSEMICARBAZONE DERIVATIVES BY USING BOVINE VIRAL DIARRHEA VIRUS AS A MODEL OF HEPATITIS C VIRUS

Wahid M. Basyouni (1), Khairy A.M. El-Bayouki (1), Samir Y. Abbas (1), Mostafa K. El-Awady (2)

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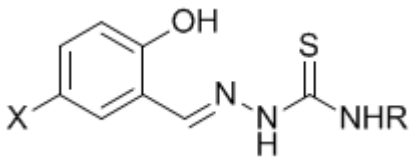
The infection by the hepatitis C virus (HCV) is a major global public health problem in the world. Hepatitis C virus is a viral pandemic and a leading cause of chronic liver disease and responsible for 350,000 death cases annually. Thiosemicarbazones were the first antiviral compounds recognized to have broad-spectrum antiviral activity against a range of DNA and RNA viruses. Where, the use of *N*-methylisatin-ß-thiosemicarbazone (methisazone) as an effective antiviral drug in the chemoprophylaxis of smallpox virus was demonstrated early.

Identification of new therapeutic agents for the treatment of viral diseases represents an area of active investigation. In an effort to develop new antiviral compounds, a series of novel 5-(arylazo)salicylaldehyde thiosemicarbazone derivatives were synthesized. These derivatives were structurally characterized using severalspectroscopic techniques and evaluated against bovine viral diarrhea virus as a model of hepatitis C virus. Some tested derivatives showed potent anti-bovine viral virus activity.

So, this result determines the potentiality of these thiosemicarbazones as antiviral agents for treating infections caused by other highly related members as hepatitis C virus.



Acknowledgement:
This work was supported by STDF, Egypt.

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O-23

Conjugated Molecule: Substituent directed light induced properties and medicinal activities

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Donor-acceptor conjugated molecules play important role in many areas of biology, chemistry, medicine and electronic device applications. Thus, newer molecules with varied light induced as well as medicinal properties are intriguing to the researcher. In addition to that, studies on the photophysical, photochemical and photobiological properties on newer molecule provide most valuable information about the structure and properties of conjugated molecule and in designing future molecule with efficient medicinal properties. In this context, we have synthesized several donor-acceptor *p*-phenyl substituted ethenyl systems and studied their substituent dependent light induced fluorescence and photoisomerization properties, medicinal activities such as antifungal and antioxidant activities and interaction with protein like bovine serum albumin. In addition to that a possible mechanism for photo reactivity of conjugated molecule, and designing of future molecules for antioxidant activity and other fields will also be discussed.

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O-24

GRAPHENE OXIDE SILVER NANOPARTICLES NANOCOMPOSITE: A MULTIFUNCTIONAL MOLECULES

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Graphene has been extensively used for cancer therapy because of its unique properties. The use of graphene to target and eliminate cancer stem cells (CSCs) is an alternative approach to conventional chemotherapy. CSCs are able to surviveconventional chemotherapy. Thus, there is an urgent need for novel approaches to CSC therapy. In this study, biomolecule-mediated reduced graphene oxide-silver nanoparticle nanocomposites (rGO-Ag) were designed and synthesized using R-phycoerythrin (RPE) as a reducing and stabilizing agent. The anticancer properties of RPE-rGO-Agwere evaluated in human ovarian cancer cells and ovarian cancer stem cells (OvCSCs).The synthesized RPE-rGO-Ag nanocomposite (hereafter referred to as rGO-Ag) was characterized using various analytical techniques. OvCSCs were isolated and characterized using fluorescence activated cell sorting (FACS). The anticancer properties of the rGO-Ag nanocomposite were evaluated using a series of cellular assays.The inhibitory effect of rGO-Ag on the growth of ovarian cancer cells and OvCSCs wasevaluated using a clonogenicassay. The expression of apoptotic and anti-apoptotic genes was measured by real time quantitative reverse transcriptase polymerase chain reaction (qRT-PCR). The prepared rGO-Ag nanocomposite showed significantly greater cytotoxicity towards both ovarian cancer cells and OvCSCs than graphene oxide, reduced graphene,and oxide and silver nanoparticles. Following 3 weeks of incubation of OvCSCs with the rGO-Ag nanocomposite, the number of A2780 and $ALDH^{+}CD133^{+}$colonies was significantly reduced. Further, the toxicity of the rGO-Ag nanocomposite was due to aloss of mitochondrial membrane integrity and enhanced expression of apoptotic genes,leading to adverse changes in the mitochondrial function and possibly triggering apoptosis.The prepared rGO-Ag nanocomposite showed significant cytotoxic potential in human ovarian cancer cells and OvCSCs, particularly with the specific $ALDH^{+}CD133^{+}$ subpopulation of cells. These findings suggest that rGO-Ag could be a novel nanotherapeutic molecule for the specific targeting and elimination of CSCs.

Keywords: Graphene; antibacterial, anticancer; nanomedicine; nanotherapy

O-25

Layered double hydroxide/ metal organic framework nanocomposites for adsorptive removal of anionic dye

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Synthetic dye removal from common water contaminant is a major issue to improve human health and environmentally sustainable development. Among various techniques, adsorptive removal is regarded as extensive method because of their merits of high efficiency, low operation cost, and easy regeneration with low secondary products. Here we report the synthesis of new nanocomposite adsorbent materials based on layered double hydroxide (LDH) and metal organic framework (MOFs) by simple solvothermal method. The organic linker anions intercalated LDHs were treated with Cu (II) ions to produce Cu based MOF nanocrystals through a bridging bidentate mode. The MOFs were deposited on the hydrophilic LDH sheets. The structures and morphology of the obtained materials were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), UV-visible and photo luminescent spectroscopy, Fourier transformation infrared spectroscopy (FTIR) and thermogravimetric analysis (TGA). The adsorption characteristics of the synthesized materials showed the best dye removal efficiency over 99% in less than 20 min with an absorption capacity of 700 mg/g. The results suggested that LDH/MOF nanocomposites could be employed as an efficient and selective adsorbent material for the removal of anionic dyes.

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O-26

Enhanced CO_2 capture of chitosan-zeolite composites for environmental applications

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Abstract

An environmental pollution is a serious problem to our ecosystems due to the rapidity of the industrialization process. Carbon dioxide (CO_2) is one of the greenhouse gases whose increasing concentration in the atmosphere. Zeolites have wide applications due to the specific chemical composition and unique porous structure. Chitosan polymer has reactive functional groups amino at C-2 and hydroxyl at C-3 and C-6 position on its backbone with acetamido groups. An attachment of amine functional groups onto high surface area of zeolite may help to advantage of high surface area and high selectivity to carbon dioxide. We have developed a simple eco-friendly procedure using chitosan to prepare chitosan/zeolite composites by solvent exchange and calcinations. The chitosan/zeolite composites were characterized by ATR-IR, XRD, TGA, SEM and nitrogen adsorption-desorption isotherm. Chitosan/zeolite composites showed enhanced CO_2 adsorption due to its mesoporous structure. Our findings are encouraging as the chitosan/zeolite composites can be used as a potential tool for environmental applications.

Acknowledgments: This research was supported by the KU Brain Pool 2017 of Konkuk University, Seoul, Korea and FCT Portugal

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O-27

Electrodeposition of polythiophene on self assembled molecular films of mercapto and methyl mercapto derivatized terthiophene

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5-mercapto 2, 2'-5", 2' terthiophene (T_3SH) and 5-methylmercapto 2, 2'-5", 2' terthiophene (T_3CH_2SH) were synthesized and purified from terthiophene. Self assembled monolayers of these compounds were formed on the freshly evaporated polycrystalline gold surfaces. Monolayers were characterized by reflection absorption infrared (RAIR) spectroscopy and electrochemical methods. It is understood from the RAIR spectroscopic data that SAMs of T_3SH exhibits a slanted orientation with a tilt angle from the surface normal, where as the T_3CH_2SH molecules found to orient vertically in their SAMs on gold surface. The surface concentration, Γ calculated using the charge passed during the reductive desorption of the SAMs is found to be 5.88 x 10^{-10} moles/cm^2 and 9.2 x 10^{-10} moles/cm^2 respectively for T_3SH and T_3CH_2SH. Electropolymerization of the bithiophene on the SAMs of T_3SH and T_3CH_2SH was carried out. The thick and dense electrochromic films of polythiophene were characterized. Appreciably thicker films of polythiophene were found to be deposited on T_3SH and T_3CH_2SH than on bare Au and C_{16} thiol modified Au electrodes.

Key words: terthiophene, polythiophene, SAM, electrodeposition.

O-28

Pulling of DNA: Emergence of new structural polymorphs and S-DNA

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Single molecule force spectroscopy measurements [1,2,3] of DNA reveal changes in DNA structure in presence of external force and around 65-70 pN forces it exhibits a mechanical transition where its extension increases by 70%. Inspite of many experimental and theoretical studies over more than a decade, there remains a significant debate on the characteristic properties of the overstretched DNA. Using extensive all atom molecular dynamics simulations we report that in the overstretched regime ds-B-DNA adopts a new elongated S-DNA [4,5,6] structure when it is stretched along the 3' directions of the opposite strands whereas stretching along 5' directions of the opposite strands leads to force induced melting form of the DNA. We next discuss the structural polymorphism of DNA exhibited through various conformations with a change in the known helical parameters. We further perform the structural characterization of the S-DNA by calculating various helical parameters. S-DNA is further characterized by changes in the number of H-bonds, entropy and free energy. We next find that the free energy barrier between the canonical and overstretched states of DNA is higher for the same termini pulling protocol in comparison to all other considered here. Our observations [5] not only reconcile with the available experimental findings qualitatively but also enhance the understanding of different overstretched DNA structures.

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O-29

Method Developed through Design of Experiments (DOE) for the Prediction of Rate Constant and Reaction Kinetics

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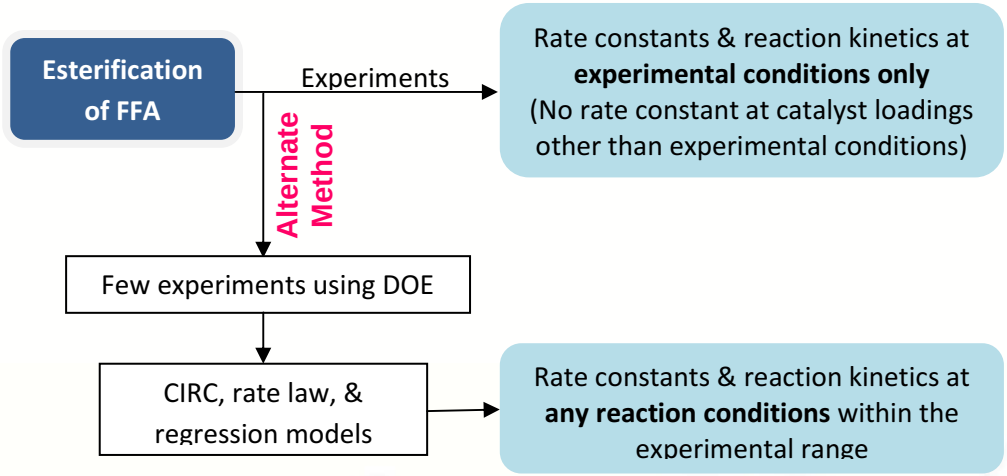
Abstract: Kinetics of a known reaction cannot be computed unless the values of rate constant are known. Rate constants are determined usually by performing experiments at different reaction conditions. In this work, a novel method is proposed for the prediction of rate constants and kinetics for sulfuric acid-catalyzed esterification of free fatty acid (FFA) with methanol for the synthesis of fatty acid methyl esters (FAME or Biodiesel) from the low-cost feed-stocks. This method is based on a concept of concentration independent rate constant (CIRC) reported by Hassan and Vinjamur (2014). Effects of catalyst loadings (0.5 – 2.0 wt%), temperature (40 – 60 °C), and molar ratio (3 – 9) on the kinetics are analyzed using Taguchi L9 (3^4) orthogonal array and full factorial (3^3 and 5^3) design of experiments. The reaction kinetics is found to be followed reversible 2^{nd}-order rate law. Conversion of FFA increases with catalyst loading, temperature and molar ratio. Regression models developed for the predictions of kinetics are statistically and kinetically tested. Model adequacy check through the residual plots assessment showed that the fitted models are well suited to regression analysis. The kinetics of reaction predicted from the regression models are well fitted to the reversible 2^{nd}-order rate law. The CIRCs estimated from the predicted kinetics are compared with the experimental values of CIRCs and most of them are found to be within ±10%.



Keywords: Esterification, Concentration independent rate constants, Reaction kinetics, Design of experiments (DOE)

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O-30

Detection of Antagonistic properties of different fungus synthesized silver nanoparticles against Gram negative bacteria's

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Abstract:

The present study indicates polydisperse spherical, ellipsoidal and 10- 70 nm sized silver nanoparticles have considerable antagonistic properties comparison with the standard anti-microbial drug.These silver nanoparticles were synthesized by 12 different fungi like as *A. alternata*, *A. flavus*, *A. fumigatus*, *A. niger*, *F. oxysporum*, *H. tetramera*, *M. phaseolina*, *P. glaucum*, *P. chrysogenum*, *T. asperllum*, *T. harzianum* and *T. viride.* These mycosynthesized silver nanoparticles were characterized by Visual analysis, UV-Vis absorption spectroscopy and Transmission electron microscopy (TEM). The silver nanoparticles exhibited maximum absorbance in between 400-480 in UV Vis spectroscopy. Agar well diffusion technique was used for the detection of antagonistic properties of these mycosynthesized silver nanoparticles against *Escheriscia coli*,*Klebsiella pneumonia* and *Pseudomonas aeruginosa* withstandard drug streptomycin. *P. chrysogenum* synthesized silver nanoparticles shows the 1.8 cm and 1.7 cm zone of inhibition against *E. coli* and*K. pneumonia* which was largest among the all fungi while as 1.7 cm zone of inhibition observed in *T. viride* synthesized silver nanoparticles against *P. aeruginosa*. Therefore this result shows that all the mycosynthesized silver nanoparticles have potent antagonistic properties against gram negative bacteria so it deserving further investigation for clinical application.

Key words- Antagonistic properties, UV Vis spectroscopy, Transmission electron microscopy (TEM), *Escheriscia coli,Klebsiella pneumonia*, *Pseudomonas aeruginosa.*

O-31

A facile synthesis of tetrahydrobenzo[*a*]xanthene-11-ones accelerated by whole cell biocatalyst, Baker's yeast

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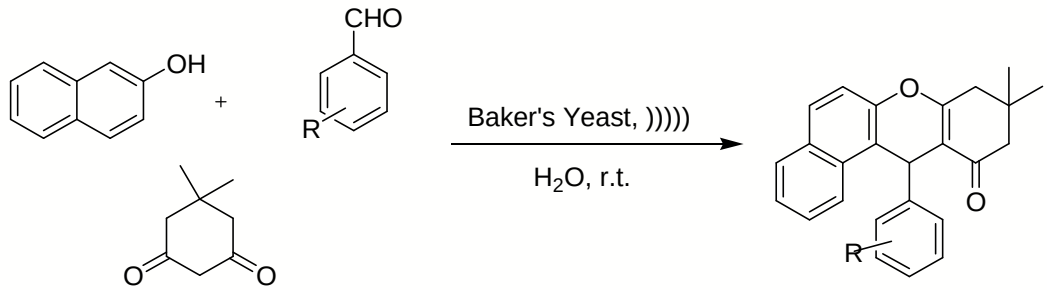
First time an efficient and greener protocol for the synthesis of bioactive12-aryl-8,9,10,12-tetrahydrobenzo[a]xanthen-11-ones has been developed,allowing a cyclocondensation of aryl aldehydes, 2-napthol and dimedoneusing readily available whole cell biocatalyst,Baker's yeast(*Saccharomyces cerevisiae*) at room temperature. The role played by ultrasonication in accomplishing the cyclocondensation has also been determined. This novel protocol is eco-friendly and cost effective. The details of the optimisation and advantages of the protocol than those already practicedwill be debated.



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O-32

Congo-Red-inspired-azo-stilbene molecular frameworks designed for metal-chelation therapy in Alzheimer's disease

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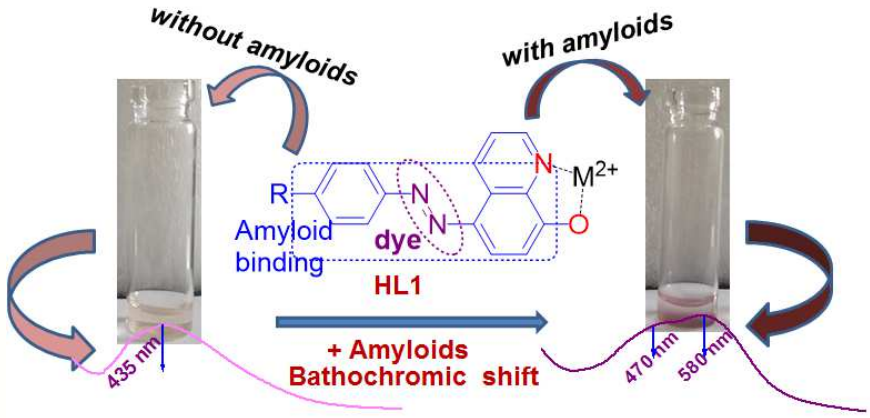
ABSTRACT

Chemical tools are needed to discover new effective drugs for tackling multifaceted complex neurodegenerative diseases like Alzheimer's disease (AD). Multifunctional nature of two compounds, 5-((4-nitrophenyl)diazenyl)quinolin-8-ol (HL1) and 4-((4-nitrophenyl)diazenyl)benzene-1,3-diol (HL2) has been investigated w.r.t. their ability to bind Cu^{2+} ions and amyloid aggregates related to AD. HL1 and HL2 have half-congo-red type azo-stilbene structural framework incorporated with metal chelating groups, designed to chelate metal ions from metal-amyloid species. Metal binding studies of HL1 and HL2 are established by the methods of Job's Plot, UV-vis spectra with metal ions and stability constant determination. In addition, their metal complexes are isolated, spectroscopically characterized and their structural analyses were obtained from DFT based calculations including binding energy determination. Amyloid fibril binding ability was established by using UV-vis spectroscopy and direct staining of amyloids. HL1 is found as an excellent colorimetric sensor for amyloids. Lysozyme protein from chicken egg white (CEWL) was used as a model peptide for fibrillation studies and conditions were optimized for its aggregation. Inhibitory effect of HL1 and HL2 and their isolated metal complexes L1-Cu and L2-Cu on CEWL fibrillation was studied using ThT and ANS fluorescence assay. Overall, these results suggest that this new class of multifunctional small molecules that can interact with amyloids as well as metals and could be potential theranostic agents to be investigated further for AD.



O-33

Invitro release study of Camptothecin from functionalized Mesoporous silica materials

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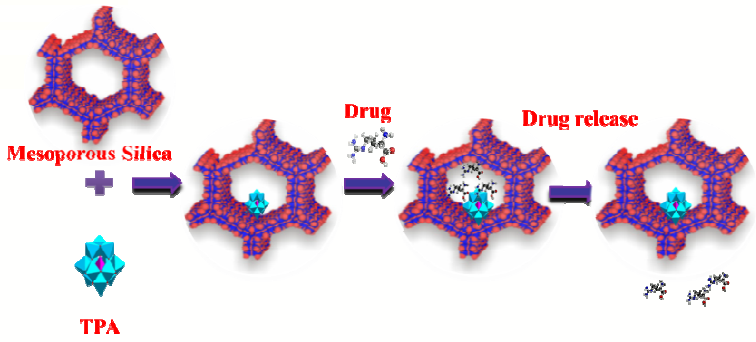
Abstract

Camptothecin (CPT) is a naturally occurring quinolone alkaloid which shows significant anticancer activity with a broad spectrum of human malignancies and CPT is an inhibitor of the DNA-replicating enzyme topoisomerase-I. Unfortunately, the clinical application of CPT is hindered by its poor pharmaceutical profile, with extreme aqueous insolubility, low stability of the lactone form at physiological pH, and severe systemic toxicities which included myelosuppression, vomiting, diarrhoea, and hemorrhagic cystitis. The mentioned problem can be overcome by using proper delivery systems. Mesoporous silica materials have gained much attraction in the field of drug delivery as they have several attractive features for controlled release. To control the release rate of drug, these mesoporous silica materials have been functionalized by various organic groups.The present paper deals with the functionalization of MCM-41 and MCM-48 using 12-tungstophosphoric acid (TPA). TPA-MCM-41 and TPA- MCM-48 have been selected to study the controlled release of Camptothecin.



In present paper, the synthesis, functionalization of mesoporous silica (TPA-MCM-41 and TPA-MCM-48), encapsulation of Camptothecin and their characterization using variousphysicochemical techniques as well as cytotoxic study will be described. MTT study was carried out using Human hepatocellular liver carcinoma (HepG2) cells. In vitro controlled release of Camptothecin was carried out in simulated body fluid, at body temperature, under stirring as well as static condition. Investigation of release kinetic and mechanism was also carried out using first order release kinetic model and Higuchi model.

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O-34

Prolonged exposure to industrial pollutants induce oxidative stress in humans

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Introduction: Heavy metals are among the industrial toxic agents detected in the environment. They have carcinogenic and cell-transforming potential. Occupational and environmental exposure to heavy metals causes toxicity in living organisms. Interaction between air pollutants and living tissues may cause disturbance of pro-oxidants and anti-oxidants in the body that may lead to tissue injury.

Objective: Industrialization causes adverse affects on human population and ecosystem. This study was done to find the effect of long term heavy metal exposure on human health.

Methods: In the present study human serums were used as bioindicator of metal toxicity and oxidative stress. Serum of group of workers from glass bangle making industry and healthy subjects were analysed for their cadmium, lead, nickel, antioxidant enzymes (indicator of antioxidant defence), alpha-1 antitrypsin levels (an enzymatic biomarker of oxidative stress. GPx activity was measured by method of Paglia and Valentine (1967). SOD was assayed by the method of Beauchamp and Fridovich (1971). Its activity was measured by the method of Waheed and Salahuddin (1975).

Results: The levels of all the three heavy metals and alpha-1 antitrypsin were found to be increased in heavy metal exposed human subjects as compared to healthy ones. However, the levels of antioxidant enzymes were found to be decreased in them.

Conclusion: The results indicated that prolonged exposure to heavy metals such as nickel, cadmium and lead caused adverse health effects. This was due to induction of oxidative stress.

O-35

Design and synthesis of linoleic acid peroxidation inhibitors of morpholine-connected pyrazolidine derivatives induced by effective antimicrobial activity

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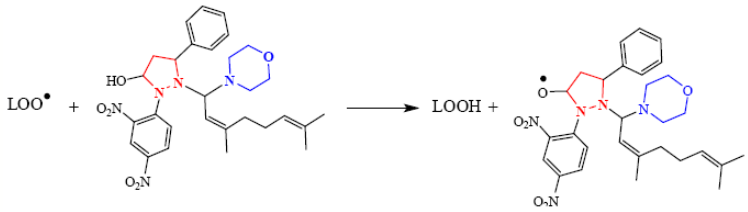
A simple and convenient one-pot four-component synthesis of morpholine-connected pyrazolidine derivatives were developed using direct metal-free catalysis (chiral pyrrolidine-based catalyst)[1-3], with the identities of the synthesized compounds confirmed by IR, NMR (^{1}H and ^{13}C), mass spectrometry, and elemental analysis. The prepared compounds were inspected for antimicrobial, antioxidant, and cytotoxic activities. Antimicrobial and antifungal activities against five bacterial and four fungal pathogens, respectively, were investigated using the disc diffusion technique. In antibacterial activity, compounds exhibited significantly higher activity (MIC = 2 µg/mL) than the standard ciprofloxacin. The results of antifungal assay showed that the activity of compound was significantly higher (MIC = 0.5 µg/mL) than the standard clotrimazole. Linoleic acid peroxidation was screened based on radical scavenging and performance[4]. Some of compound showed substantial antioxidant (91.3%) activities, as compared with the Trolox standard. Cytotoxicity[5] was evaluated using HepG2 (liver), HeLa (cervical), and MCF-7 (breast) cancer cell lines, with high toxicities observed (GI_{50} = 07.8 µm to 12.2 µm).



Linoleic acid peroxidation

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O-36

Synthesis and Biological evaluation of pyrazolopyrimidine and pyrazolopyridine derivatives

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Abstract:

The heterocyclic scaffolds have been found to be excellent drug intermediates are extensively studied and referenced in literature. [1-4] Among allof the heterocyclic compounds, pyrazole fused pyrimidine show diverse pharmacological activities such as antiviral [5], anti-HIV [6], antibacterial [7,8] andespecially anticancer agents. [9,10] Pyrazolopyridines also show diverse biological activities such as antibacterial [11], antiviral [12] and antimalarial agents [13].Novel pyrazole fused pyrimidines, pyridines and pyrazoles were designed and synthesized by an efficient one pot method with good to excellent yield. The synthesized compounds were tested for antibacterial and antifungal activities and also evaluated for their anticancer activity against two cell lines. (K562, A549)

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O-37

Fe_3O_4 Embedded NH_2-MIL 125 (Ti) MOF Composite for Selective and Efficient Removal of Aqueous Lead

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ABSTRACT

Aquatic remediation by Metal–organic frameworks (MOFs) has been proved to be an efficient latest technology. To design MOFs with both good stability and quick recyclability is still a critical challenge. In this study, a stepwise embedded Fe_3O_4 nanoparticle on the surface of NH_2-MIL-125 (Ti) was successfully employed and applied to aquatic remediation. The characterization results reveal that the composite elucidates excellent saturation magnetization value of 59.3 emu g^{-1} with high specific surface area 650 m^2 g^{-1} and a pore size of 5 nm. The obtained TEM and HRTEM images illustrate that the Fe_3O_4 nanoparticles were uniformly embedded onto the surface of MOF and the TGA demonstrated the high thermal stability of the composite. The composite was employed for quick and immense removal of Pb(II) from aqueous solution. The effect of various parameters like pH, contact time, initial metal ion concentration, interfering ions and temperature on the adsorption capacity of the nanoporous composite were examined. The Langmuir model presented the best fitting with a maximum adsorption capacity up to 769 mg g^{-1} at pH 5 and 298 K. Moreover, by increasing the Fe_3O_4 precursor on nanoporous NH_2-MIL-125 (Ti) decreased the recovery time (15 sec) in adsorption process, and the same can be recycled 7 times without apparent loss of the adsorption capacity of Pb(II) in water, which is significantly pave for its future practical treatment of industrial waste discharge.

Keywords: Fe_3O_4; NH_2-MIL-125 (Ti); XPS; Pb(II) removal; recycle

O-38

GREEN SYNTHESIS OF NOVEL SPIRO NITROGEN AND SULFUR CONTAINING HETEROCYCLES AND THEIR ANTI-INFLAMMATORY ACTIVITY

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Compounds with spirocyclic structures having one common sp^3 carbon atom between two rings an interesting synthetic challenge due to their important structural rigidity and complexity. Numerous spiro compounds have been collected from plants and animals serve as important synthones in drug design and synthesis. Spiro heterocycles containing nitrogen, oxygen and sulfur atom have shown notable roles in biological processes and exhibited significant pharmacological activities. Further, construction of hybrids of two active pharmacophores has been considered as better approaches to achieve more biological active targets.

Now days, considerable awareness has been focused on the development of green, well-organized and eco-friendly chemical processes using heterogeneous solid catalysts to synthesize drugs like compounds. Keeping in view of above all and in connection with our previous research focused on ecofriendly synthesis of heterocyclic compounds novel spiroheterocyclic hybrid has been synthesized by comprising various biological active moieties such as indeno[1,2-*b*]quinoxalinone, thiazolidinone, isoxazole and indole-2,3-dione in a single molecular structure using efficient and eco-compatible approaches. The anti-inflammatory activities were also studied for these spiro compounds using acute carrageenan-induced paw edema model in rats.

The details of present work and mechanism will be discussed during the conference.

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O-39

Rheological behavior and Ibuprofen delivery applications of pH responsive composite alginate hydrogels

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Abstract

Synthesis and structural characterization of hydrogels composed of sodium alginate, polyethylene oxide and acrylic acid with cyclodextrin as the hydrocolloid prepared at different pH values is presented. The hydrogels synthesized show significant variations in rheological properties, drug encapsulation capability and release kinetics. The hydrogels prepared at lower pH (pH 1) are more elastic, have high tensile strength and remain almost unaffected by varying temperature or frequency. Further, their Ibuprofen encapsulation capacity is low and releases it slowly. The hydrogel prepared at neutral pH (pH 7) is viscoelastic, thermo-reversible and also exhibits sol–gel transition on applying frequency and changing temperature. It shows highest Ibuprofen encapsulation capacity and also optimum drug release kinetics. The hydrogel prepared at higher pH (pH 12) is more viscous, has low tensile strength, is unstable to change in temperature and has fast drug release rate. The study highlights the pH responsiveness of three composite alginate hydrogels prepared under different conditions to be employed in drug delivery applications.

O-40

An Effective Approach for Enhanced Recovery of Oil using Polymer-Nickel Nanoparticles Mixture

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ABSTRACT

Crude oil is recovered by two different process i.e., primary and secondary recovery. Primary recoveryutilizes the resident geological pressure for producing oil. As pressure decreases, secondary recovery is done by water flooding to re-pressurize the reservoirs and sweep the oil towards production well. Thiseventually loses its efficiency in recovering oil with increasing water to oil ratio.At this point, a tertiary process, also known as enhanced oil recovery (EOR)is implemented to increase oil production. In this study we have tried injection of nickel nanoparticles along with a biopolymer xanthan gum to alter the rock wettability, lower interfacial tension and increase sweep efficiency for recovering additional oil.Initially the rheological properties of xanthan gum dilute solutions prepared with different solvent system were assessed. It was found that the decrease in intrinsic viscosity for xanthan gum solution prepared in brine and nanoparticles containing medium were comparable reflecting the suitability of using a polymer nanoparticle mixture. Oil containing sand pack bioreactors were used to evaluate the production of additional oil when nanoparticle and polymer solution was injected.Results indicated the production of additional oil with nanoparticle and polymer mixture of about 5.93 % of residual oil in place compared to 4.48 and 4.58 % using polymer and nanoparticles respectively. Ogolo et al. [1] had conducted similar flooding test withdifferent nanoparticles and had shown 5% additional recovery using aluminium oxide nanoparticles. The flooding experiments thus shows the potential of the mixture of nanoparticle and polymer as a better recovery agent.

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O-41

Natural sunscreen development from cyanobacterial isolates of hypersaline environments of India

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Abstract

Ultraviolet radiation (UVR) is harmful to living system; causing damage to biological macromolecules. Available inorganic and organic chemicals used in commercial sunscreen have deleterious activity *in vivo*. Therefore, there is need of safe and natural sunscreen[1].Aunique and green strategy for dealing with UV exposure is the biosynthesis of mycosporine-like amino acids (MAAs) by several organisms. MAAs are the most common group of UVRabsorbing intracellular secondary metabolites with a maximum absorbance between 310 and 362 nm[2]. These molecules have wide phylogenetic distribution. Among them, cyanobacteria are the impressive source of these MAAs that can be exploited industrially[3].MAAs primary function is photo-protectant but they are also potential osmolytes[4]. Keeping this in mind, we collected samples from hypersalineSambharlake, Jaipur, Rajasthan. From these samples, pure cultures of*Arthrospira* sp. and *Anabaena* sp. cyanobacteria were isolated. Isolates werethen induced by UV-B for MAAs production. We find that crude methanolic extracts of induced samples have UV absorbing range from 330 to 350 nm, with characteristic peak at ~340 nm. This peak might correspond the production of porphyra-334 or shinorine by these cyanobacterial isolates under UV stress.*Arthrospira* type isolates have UV absorbing peak till 36 hrs UV-B induction periods, while *Anabaena* have till 48 hrs. In conclusion, present work revealed the presence of potential MAAs in cyanobacterial isolates of hypersaline environments of India. Future perspectives include search for other MAAs and then co-production of these different UV protective molecules in order to develop broad spectrum natural and safe sunscreen.

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O-42

Green Synthesis of Zinc Nanoparticles using *Ipomoea asarifolia*Leaves Extract and its Application for Dyes Removal

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Abstract

The green synthesis of zinc nanoparticles using *Ipomoea asarifolia* (Swamp Morning Glory) leaves and its application for dyes removal was reported. The synthesised NP was characterised using FTIR, SEM and XRD which was found to be crystalline with an average particle size of 39.15nm. From batch adsorption studies the NP was found to be efficient in removing the dyes with a high affinity of Eriochrome Black T compared to the remaining two; for which %R varies as 90.31%, 81.98% and 89.56% for EBT, IY and BPB at their respective optimum pH values. The adsorption of the dyes were all found to be physisorption process.

Keywords Zinc Nanoparticles, Adsorption, Dyes, Green Synthesis

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O-43

Study of Aggregation Kinetics of Macrocyclic Polyammonium Cations Guided Aggregation of Citrate Capped Silver Nanoparticles

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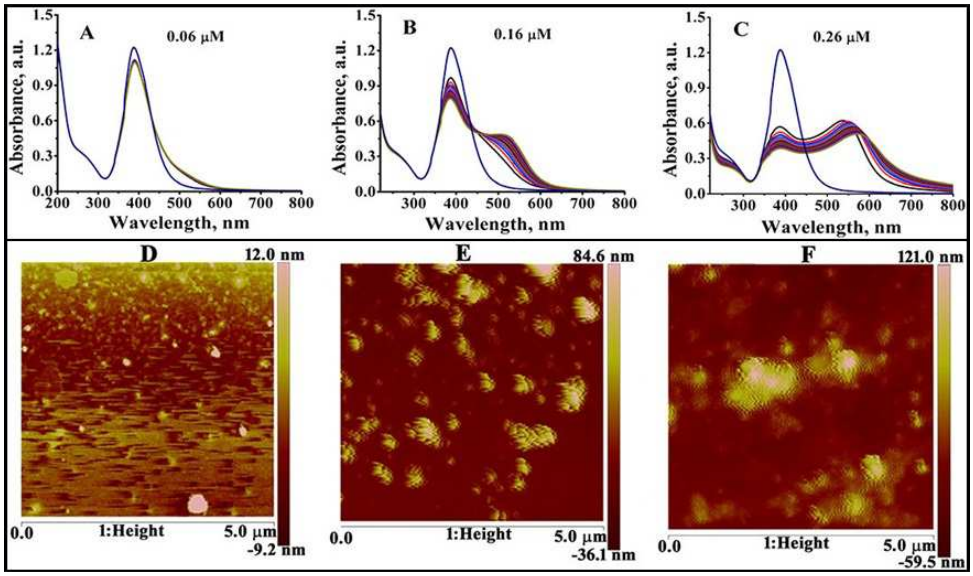
Abstract: The study would provide the insight of molecular interactions involved in nanoparticle surface-adsorbed anions with biological polyamines. We have studied aggregation of citrate capped silver nanoparticles (cit-Ag-NPs) in presence of macrocyclic polyammonium cations (MCPACs): Me_6[14]ane-$N_4H_8^{4+}$(Tet-A/Tet-B cations) and [32]ane-$N_8H_{16}^{8+}$ Misra et al.[1,2],which are well reputed anion recognizers and are treated as to mimic of biological polyamines. The ultraviolet–visible time-scan plots over the reduction of the absorption band of surface plasmon resonance of cit-Ag-NPs at 390 nm are well fitted with fourth-order polynomial equation and are employed to determine the initial aggregation rate constant Moskovits [3].The evaluated H-bonded association constant (K_{asso}) using Benesi–Hildebrand method reveals that [32]ane-$N_8H_{16}^{8+}$cations form stronger association complex, as expected, with the citrate anions than the Me6[14]ane-$N_4H_8^{4+}$cations.



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O-44

Synthesis and biological properties of palladium complexes

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Complexes with biologically active ligands are particularly attractive, as they combine qualities of classic non-targeted coordination compounds and organic ligands which offers much scope for the design of novel drugs with enhanced, targeted activity[1]. DNA is an important cellular receptor andmany chemicals exert their pharmaceutical properties by binding with DNA thereby changing the replication of DNA and inhibit the growth of the cells which is the basis of designing new and more efficient drugs and their efficacy depends on the mode and affinity of binding[2].Binding studies of small molecules andDNA are very important in the development of DNA molecular probes and new therapeutic agents.

Palladium complexes stabilized by a chelate or a strongly coordinated, bulky nitrogen or oxygen donor atoms are known to be of high biological importance such as antitumor, antibacterial and antifertility properties [3].

In view of this, a number of palladium complexes were synthesized. The square planar geometry around palladium with O, N, and S donor atoms was confirmed by X-ray crystal structure. These palladium complexes were found to inhibit the growth of bacteria and scavenge free radicals efficiently. These complexes also strongly bind to DNA via groove binding and the thermodynamic parameters suggest that hydrogen bonds play a predominant role in the binding of complexes to DNA.

Keywords: Palladium, diarydisulfides, DNA binding, anti-oxidant

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O-45

Synthesis and characterization of substituted Mo and W carbonyl complexes containing isoniazid and dimethylglyoxime

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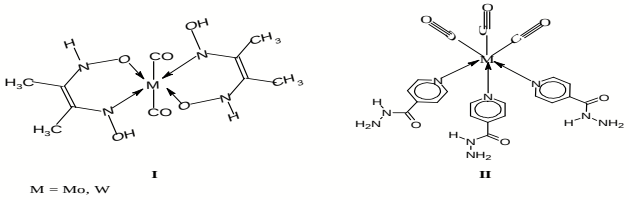
Substituted metal carbonyls with biologically relevant ancillary ligands are reported to systematically release CO and non-harmful substrates *in vivo* promising to be useful candidates as CO-releasing molecules (CO-RMs) [1]. In a one pot synthesis, we prepared substituted carbonyl complexes of dimethylglyoxime (DMG) and isoniazidusing manipulated Schlenk technique under N_2 in THF. The decarbonylation and substitution of the Mo & Whexacarbonyls were successfully carried out by stirring the mixtures at room temperature for 24 h and 36 h respectively in the presence of trimethylamine N-oxide.The compounds were characterized using ^{1}H NMR, FTIR, and CHN analyses. Results reveal dicarbonyl and tricarbonyl species**I** and **II**, where two DMG and three isoniazid moieties were coordinated to the central metal atoms.



I **II**

The resulting complexes with CO ligands of decreased bond strength promises to be good candidates for CO release studies in biological system with the use of appropriate CO release activating agent, thus offering some hope for their use as CO-releasing molecules.

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O-46

Thermokinetic of poly(3-hydroxybutyric acid)(PHB) batch production by Azotobactervinelandii

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Bioplastics production from microbial sources is an emerging area which even provides opportunities to convert wastes into bioplastics. Poly (3-hydroxybutyric acid) (PHB) a well- known bioplastic which is stored as intracellular cytoplasmic inclusion bodies as a biopolymer in microorganisms. PHB is the sustainable alternative to the conventional plastic due to their biodegradability. The objectives of this study were to monitor the PHB production using *Azotobactervinelandii* and evaluatethe thermo-kineticdata in a bio-reaction calorimeter (BioRC1e) in real time. Bio- calorimeter online real-time measurements provide a direct evaluation of the performance robustness of the bacterial system. The metabolic heat generated during these investigations in a batch reactor (BioRC1e) was found to be incorrelation with the biomass formed, substrate consumption, Oxygen Uptake Rate (OUR), Carbon-di-oxide Evolution Rate (CER) and PHB production. The OUR pattern explains the aerobic nature of the *Azotobactervinelandii* in the batch mode of operation. The accurateand reliableheat yieldvalues of complex biological reaction system through bio-reaction calorimeterprovide insightintothe metabolic processes of the *Azotobactervinelandii*. The Dry cell weight (DCW) and PHB concentration were found to be 7.2 g/L and 3.5 g/L respectively at the end of thebatch experiment (24th h).

Keywords: Poly (3-hydroxybutyric acid) (PHB), *Azotobactervinelandii*, Bioreaction calorimeter and heat.

O-47

SYNTHESIS AND EVALUATION OF SOME NEW COMPLEXES OF 6-METHOXY-3FORMYLCHROMONE WITH COPPER (II), COBALT (II) AND ZINC (II) AS POTENTIAL ANTIMICROBIAL AGENTS

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A new series of Cu (II), Zn (II) and Co (II) complexes have been synthesized from 6-Methoxy-3-phenyliminomethylchromen-4-one, a Schiff base derived from 6-Methoxy-4-oxo-4Hchromene-3-carbaldehydeand aniline. The nature of bonding and the structure of the complexes have been deduced from IR, UV, 1H NMR spectroscopy. The biological activity of the ligand and metal complexes have been examined against both gram-positive as well as gram-negative bacteria by the Agar well method using DMSO as solvent and Gentamicin as standard drug. The zone of inhibition values and MIC were measured at 37 ºC for 24 h. Antimicrobial screening tests displayed better results for the metal complexes as compared to the ligand.

Keywords: 6-Methoxy-4-oxo-4H-chromene-3carbaldehyde, Schiff base, MIC, Metal complexes, Antimicrobial activity

O-48

EXTRACTION OF CELLULASE ENZYME FROM TOMATO FRUITS AND PINEAPPLE PEEL USING *ASPERGILLUS NIGER* AND ITS APPLICATION IN TEXTILE WET PROCESSING

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Abstract

Cellulase enzyme production by *Aspergillus niger* was studied using tomato fruits and pineapple peel as a substrates. An investigation of the various properties of the partially purified cellulase enzyme extracted from both the tomato fruits and pineapple peel deteriorated by *Aspergillus niger* was carried out in this study. The percentage yield for the two substrates was compared. The results obtained shows that the percentage yield from pineapple peel was greater than that of the tomato fruits, and the pH, temperature and the substrates concentrations have great effect on the activity of the cellulase enzyme on a grey cotton fabric. It was establish that cellulase treated cotton fabric had improved surface hair removal and luster, excellent dye uptake capacity compared to the unmodified (i.e. untreated) dyed cotton fabrics coupled with significant improvement in the fastness properties, respectively. Dyeings from the Reactive dye generally exhibited better dyeing properties than those from the Direct dye.

Keywords: Cellulase enzyme, *Aspergillus niger*, local substrates, textile, dye uptake

O-49

Cooperative regulation of human Exonuclease1 (hExo1) activity by 14-3-3 proteins

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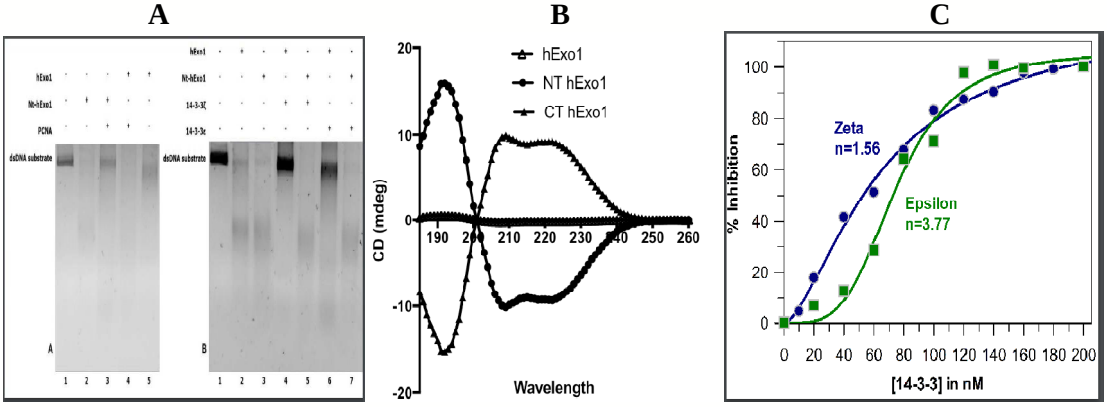
Human Exonuclease I (hExo1) mediated resection of DNA double-strand break ends generates long 3' single-stranded DNA overhangs required for homology-based DNA repair and activation of the ATR-dependent checkpoint. Despite its critical importance in inducing the overall DNA damage response, the mechanisms and regulation of the hExo1 resection pathway remain incompletely understood. Two thirds of hExo1 is predicted to be intrinsically disordered, and it is in this region that many post-translational modifications and binding events are known to occur. Many previous investigations [1, 2] have centred on the phosphorylated form of hExo1, showing a stimulatory effect on enzymatic activity by the processivity factor PCNA and 14-3-3 proteins. We have investigated the relationship between binding of partner proteins and hExo1 function in its unphosphorylated state. We have shown that there is a cooperative inhibition of the hExo1/PCNA complex by 14-3-3: the strength of the binding reaction varies with 14-3-3 isotype, and involves at least three 14-3-3 dimers.



A) 14-3-3s inhibits full length hExo1 but not Nt-hExo1 resection activity.
B) Far CD spectra of hExo1 (open triangles) and NTD-hExo1 (black circles). By deducting the two spectra it is possible to calculate the spectra of CTD-hExo1 (black triangles).
C) Binding curve. Allosteric inhibition of hExo1 exonuclease activity by 14-3-3 proteins and cooperative binding of 14-3-3 proteins to hEXo1.

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O-50

Removal of nitrogenous pollutants and organic matters simultaneously from two different wastewaters using biocathode microbial fuel cell

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Microbial fuel cells (MFC) have become an attractive technology in the last decade for simultaneous wastewater treatment and bioelectricity production. In an MFC, the anaerobic bacteria at the anode biologically oxidize various substrates. The electrons generated during the microbial oxidation reaction are transferred to the anode and flow to the cathode to combine with protons and oxygen to form water. The objective of this work was to investigate the feasibility of using biocathode MFC in a continuous mode with different organic loading rates (OLR) and ammonia loading rates (ALR) in the anodic and cathodic chamber, respectively and their resulting effects on the wastewater treatment efficiency as well the power production. The experiment was designed by using the two different types of synthetic wastewaters in a dual chamber MFC. Anodic chamber contain glucose rich synthetic wastewater while ammonia rich synthetic wastewater was used in the cathodic chamber. When the cell potential was stable after 16 days of batch mode operation, the MFC was converted to continuous mode (from batch mode) and operated for 125 days with different OLR and ALR and fixed hydraulic retention time (HRT) of 40 h. The OLR of 1.49 kg COD m^{-3} d^{-1} and ALR of 0.58 kg NH_3^- m^{-3} d^{-1}, for anodic and cathodic chambers, respectively, gave the best results. The highest value of cell potential on these OLRs was 310 mV with current density of 85.11 mA m^{-2}, power density of 26.38 mW m^{-2} and volumetric power density of 192.20 mW m^{-3}. During this period, COD reduction was 78–83% in the anodic chamber and the ammonia reduction was 36–38%. After stable operation with synthetic wastewater one case study was performed with complex industrial wastewater. Continuous mode operation was performed at two different OLR and HRT with a constant ALR. A stable power density and volumetric power density of 23.56 mW m^{-2} and 112.50 mW m^{-3}, respectively were achieved after 24 days of continuous operation at an OLR of 0.35 kg COD/m^3 day with an ALR of 0.43 kg NH_3^- m^{-3} day^{-1} and corresponding HRT of 68 h. A maximum of 89% COD removal and 40% removal of ammonia was obtained after 50 days. A stable voltage of 300 mV was obtained across 1000 Ω resistance. The experimental results show that synthetic wastewater and complex industrial wastewater can be treated in biocathode MFC. The nature of microbes in both anodic and cathodic the chambers were totally different and both organics (COD) in anodic chamber and ammonia in cathodic chamber was removed along with bioelectricity production.

O-51

PLANT-METAL INTERACTIONS FOR SOIL AND WASTEWATER TREATMENT

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Interactions of plants and associated microorganisms particularly bacteria with metals in contaminated soil and water to serve as a remedial measures to metals contamination have been recognized. The soil and water resources are getting contaminated with high concentration of metals due to irrigation of agricultural field with untreated wastewater and discharge of untreated wastewater into the water bodies. Contamination and increasing level of metals in soil and water lead to effects soil microbes and aquatic biota due to their persistent nature and toxicity, therefore, quality of soil and water may degraded. Growing crops in metal contaminated soil or irrigation with contaminated water also contaminate food chain which lead to harmful effects on health of human being and other animals. Using green plants and associated microbes to remove, detoxify or stabilizing metal polluted sites have been accepted as green technique in the different countries. Several metal tolerant and hyper-accumulator plants and their interaction have been explored for removing metals and other contaminants for soil and water. Interaction of metal-plant-microbes in the rhizosphere region induce different mechanisms for defense and metal uptake in plants. Use of plants to remove metals from contaminated sites has been well documented, plants have been used for removal of metals from distillery effluent, tannery effluent, sewage and contaminated soil.Therefore, exploration of plant-metal interactions for purifying contaminated siteseither by using efficient individual plant or the combinationof plantsmay be a cost effective and ecofriendly technology over conventional methods for soil and wastewater treatment.

Key words: Metals, Phytoremediation, Wastewater, Tolerance, Hyperaccumulator

O-52

HEAVY METALS POLLUTION OF SURFACE WATER AND SEDIMENT OF WATARI RESERVOIR, KANO STATE, NIGERIA

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Abstract

Watari reservoir is one of the largest man made dams in Northern Nigeria. It was constructed for the purpose of irrigation, drinking water supply, recreation and limnology. To assess the pollution status of the reservoir, water and sediment samples were collected in three seasons of the year; November - February (cold season); March - June (dry season) and July - September (rainy season) from five sampling sites. The samples were analysed for heavy metals; Cd, Cr, Co, Cu, Fe, Pb, Mn, Ni and Zn using Atomic Absorption Spectrophotometer (AAS). The result obtained was found to be comparable to those reported for tropical reservoirs. Fe recorded the highest mean values of 6.53 mg/L in water and 12.21 mg/kg in sediment which is above the acceptable limit. Cr was BDL in water and 0.79 mg/kg in sediment. Statistical analysis shows that the values obtained in sediment were higher than those of water samples with significant difference $p<0.05$ which is due to the fact that sediments serve as sink for heavy metals. The high concentration of Fe may be due to natural origin and the presence of these metals in sediments may be an indication of anthropogenic pollution. The result of HPI, 17.98, indicates that Watari reservoir has an excellent water quality and can be used for irrigation and domestic purposes.

Key words: *Reservoir water, heavy metals, pollution, Watari reservoir, sediment*

O-53

Uncoupling of Na-H Exchanger-1 and Carbonic Anhydrase in Inflamed Colon in Experimental Colitis

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Carbonic anhydrase-I, II (CA-I and CA-II) are the major isoforms, while the CA-IV is a minor isoform in both colon and ileum. Expression level of these isoforms was significantly decreased in the trinitrobenzenesulphonic acid (TNBS) inflamed colon, whereas the level in the non inflamed ileum remained unaltered. The isoforms CA-I and CA-II, but not the CA-IV isoform were co-immunoprecipitated with the Na-H-Exchanger-1 (NHE-1) isoform suggesting an interaction between these proteins. The level of reduction seen in CA-I and CA-II proteins by co-immunoprecipitation experiments was significantly more pronounced as compared to the reduction measured by western analysis. Data from the confocal immunofluorescence microscopy also confirmed binding of both CA isoforms with NHE-1 in non colitis control colon. However, there was uncoupling of NHE-1 and CA isoforms in the inflamed colon which will allows diffusion of H^+ ions into the cytosol leading to intracellular acidification and tissue damage. Pro-inflammatory TNF-α treatment of non inflamed colonic strip ex-vivo caused a significant reduction in the level of CA-I and CA-II protein expression. Inflammationas confirmed macroscopically, microscopically, and biochemicallywas localized to the colon only, but not to the ileum. These findings suggest that reduction in CA expression in the present model is mediated by inflammation, and lack of binding of CA with NHE-1 accounts for the suppression of NHE-1 expression seen in colitis. We speculate that colonocytes from inflamed colon should have intracellular acidosis accounting for tissue damage besides diarrhea and motility dysfunction. These findings are new and adds new insights into the pathogenesis of IBD, and may be taken into consideration while designing a therapy for IBD.

Acknowledgments

Ms Verghese L and Al-Shamali A for technical support, Animal House and the Research Core Facility for animals and instrumentation. Research Sector for financial support (Grant # MB 03/15).

O-54

The potential application of aromatic and cyclic amino acid based surfactants in soap-like formulations

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Surfactants constitute of a vital class of compound which are used as active ingredients, representing 15% to 40% of the total ingredients in cleaning agents, cosmetics and detergents. Amino acid based surfactants which are considered to be a safer alternative to conventional surfactants have attracted widespread attention due to their relatively low toxicity and hypoallergenic, low irritancy, and high biodegradability.

This study involves the synthesis, physicochemical properties and biological activities of aromatic and cyclic amino acid surfactants. The synthesized surfactants displayed good antibacterial activity which was found to increase with chain length and then tail off at higher chain length, exhibiting a cut-off effect. The binding studies of the surfactants with the phospholipid 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) as model membrane demonstrated that the surfactants bind with DPPC via both electrostatic and hydrophobic interactions which have a direct effect on the antibacterial activities. The synthesised surfactants also showed selectivity towards bacterial cells rather than mammalian cells at monomeric concentration.

The physicochemical and biological properties of the synthesised surfactants in mixed surfactant systems with sodium dodecyl sulfate (SDS) or cetyltrimethylammonium bromide (CTAB) were studied in order to investigate their effectiveness in detergent formulations. The different mixed surfactant systems studied showed enhanced antibacterial properties over their single surfactants, displaying optimum antibacterial properties together with a lower ocular irritancy at particular mole fractions. Overall, evidence from this study shows that the different surfactant mixtures studied can be employed as potential ingredients in soap-like formulations due to their good antibacterial property and a relatively lower ocular irritancy.

Keywords: surfactants, phenyl alanine, tyrosine, phospholipid binding, ocular irritancy

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O-55

Nanomedicine based strategies for the treatment of Hypercholesterolemia and related Cardiovascular diseases

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ABSTRACT

Cardiovascular diseases are one of the leading causes of death worldwide that includes coronary heart disease (CHD), cerebrovascular disease, elevated blood pressure (hypertension), peripheral artery disease and other forms of heart diseases. Major cardiovascular risk factors include elevated level of blood lipids, hypertension, obesity, smoking, diabetes and reduced physical activity. It is well established that high levels of plasma low density lipoprotein cholesterol (LDL-C) i.e. hypercholesterolemia are associated with the incidence of major cardiovascular disorders, fatal and non-fatal acute myocardial infarctions and total mortality and morbidity. Statins are one the major drugs for the treatment of hypercholesterolemia. Recently, proproteinconvertasesubtilisin/kexin type 9 (PCSK9) is a secretory proprotein convertase (PC) that has been implicated as a critical regulator of LDL cholesterol. It is highly expressed in adult liver hepatocytes, secreted after autocatalytic cleavage of its zymogen form. PCSK9 interacts with low density lipoprotein receptor (LDLR) thereby leading to its degradation, resulting in the up-regulation of plasma LDL-C. Moreover, single point mutations in PCSK9 responsible for either gain-of-function (GOF) or loss-of-function (LOF) are convincingly associated with either hypercholesterolemia or hypocholesterolemia. This observation established PCSK9 as therapeutic target. Since then, several approaches have been reported for inhibiting its function, including strategies based on gene silencing by siRNA, antisense oligonucleotides, locked nucleic acids (LNA), polyclonal and monoclonal antibodies. However, the therapeutic potential of nucleic acids based approach is hampered by poor cellular uptake, rapid enzymatic degradation and the use lipid-based delivery systems. We are using nanomedicine based strategies for the development of effective, safe, target specific strategies to suppress the metabolic function of PCSK9 gene in mammalian cell culture and animal model.

Keywords: hypercholesterolemia, gene silencing, nanomedicine, nanoparticles, PCSK9

O-56

Ruthenium-Catalyzed Cascade C-H Functionalization of Phenylacetophenones.

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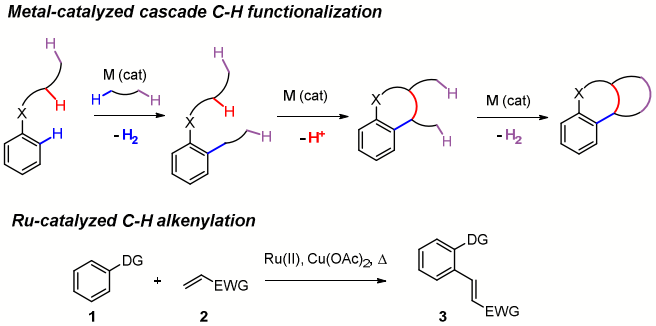
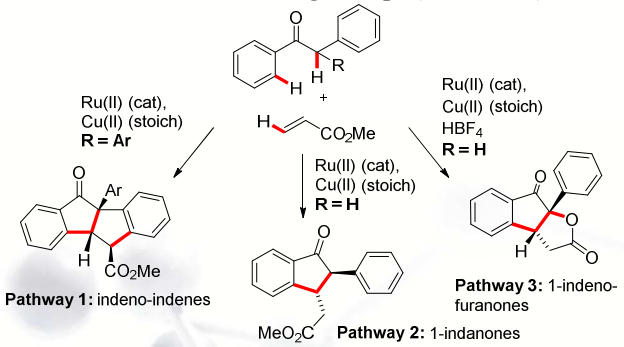
Transition metal catalyzed C–H functionalization removes the need to pre-functionalize C–H positions for C–C and C–X bond formation, enhancing both the scope and efficiency of synthetic route design.[1] The concept has great potential in the context of cascade synthesis, where an initial C–H functionalization leads to bond formation, with the new motif being primed for a second metal-catalyzed C–H functionalization (Scheme 1). Further iterations are then possible, according to substrate design, resulting in the rapid construction of complex structures with little or no requirement for pre-functionalization.[2,3]



Scheme 1 Cascade C-H functionalization.

Along the same line we have uncovered a novel cascade sequence which leads to diverse set of compounds via Ruthenium-catalysis on which we wish to present.[4] Arylacetophenones react with Michael acceptors under Ru catalysis to set up triple and quadruple C-H functionalizationpathways. Through choice of reaction conditions, novel indanone, indeno-indene carbacycles, and indeno-furanoneheterocycles can each be accessed in a single step. (Scheme 2)



Scheme 2 Ruthenium catalyzed cascade C-H functionalization.

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O-57

Synthesis of novel imidazo[1,2-a]pyridine-4-hydroxy-2H-coumarins by GBB multicomponent reaction aspotential NS5B inhibitors

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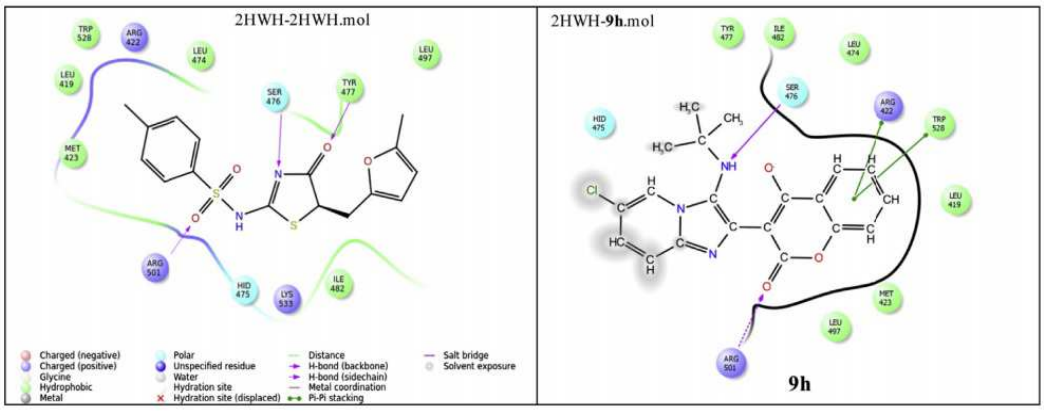
Abstract:A new series of imidazo[1,2-a]pyridine-coumarin hybrid has been developed by combining two biologically active pharmacophores coumarin and imidazo[1,2-a]pyridine following a GBB multicomponent reaction (MCR),Molecular docking studies of these novel compounds with nonstructural protein 5B (NS5B) exhibited promising binding interactions by forming hydrogenbond at Ser476, Trp528, Arg422 and Arg501, directly and hydrophobic contacts with Leu419, Ile482,Leu497, Leu489, Met423, Leu474 and His475, which are potentially useful for a new scaffold discovery.



Keyword: GBB reaction, Hepatitis C virus, 4-Hydroxy-3-Formylcoumarin, Imidazo[1,2-a]pyridine, NS5B inhibitors, Molecular docking, Multicomponent reaction (MCR).

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SYNTHESIS, CHARACTERIZATION AND PHARMACOLOGICAL ACTIVITIES OF SOME SUBSTITUTED HETEROCYCLIC COMPOUNDS

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Abstract: It has been reported in the literature that substituted 1,3,4-oxadiazole, 1,2,4-triazole, isoxazoline and pyrimidines derivatives possess significant antimicrobial activity. The Non-steroidal Anti-inflammatory Drugs (NSAIDs) are among the most commonly used drugs, but their use is associated with significant untoward effects on gastro-intestinal tract. The largest group of NSAIDs is aryl alkanoic acid class of drugs. Some well known drugs of this class are aspirin, ibuprofen, indomethacin, diclofenac, ketoprofen, naproxen etc. The major side effects in the use of these drugs are gastric ulceration and irritancy, which is partly due to corrosive nature of the carboxylic acid present in them. The aim of this study was to synthesized therapeutically effective anti-inflammatory agents, which have lesser side effects, especially hemorrhages and gastric ulceration. It was interesting to note that all the selected heterocyclic derivatives showed significant reduction in the ulcerogenic effect when compared with the standard drug ibuprofen. Among all the tested heterocyclic derivatives, 1,3,4-oxadiazoles showed maximum anti-inflammatory activity.

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O-59

Triazolium ion Based *N*-Heterocyclic Carbene Precursors: Efficient Synthesis and Photophysical Properties

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N-Heterocyclic carbenes (NHCs) derived from triazolium salts are a uinque class of organocatalysts which are primarily employed to reverse the polarity of certain functional groups. Benzoin condensation and Stetter reaction are efficiently catalyzed by triazolium salts in which NHCs behaves as an efficient nucleophilic catalyst (1). NHCs have been extensively used in the carbon-carbon bond formation *via* electrophilic "Breslow intermediate" (2). Moreover, NHCs were used in various transition metal-catalyzed coupling reactions namely Suzuki-Miyaura, Sonogashira, Hiyama and Buchwald-Hartwig (3). Formation of NHCs has received immense significance in synthetic chemistry owing to their usefulness, as a catalyst (4). On the other hand, diaryliodonium salts are versatile arylating agents in organic synthesis because of low toxicity, easy handling, recylability, high reactivity and selectivity against various nucleopliles (5). It is widely used in the construction of various crucial C-C, C-N, C-O and C-S bonds with or without transition metal-catalysts. Besides their applications in arylation reactions, diaryliodonium salts have also been successfully utilized in the assembly of medicinally important heterocyclic frameworks such as acridones, oxindoles and polycyclic quinolines in a cascade fashion (5). Due to the prominent applications of NHCs and diaryliodonium salts (6), we have developed an operationally simple and efficient protocol for the synthesis of pyrido-annulated triazolium salts in the presence of a copper catalyst. Synthesized triazolium salts were well characterized by their NMR (^{1}H & ^{13}C) and mass spectral data. Optimization of the reaction conditions, synthesis, reaction mechanism and photophysical studies of triazolium salts will be discussed during the conference presentation.

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O-60

The Effect of Temperature on Photovoltaic (PV) Efficiency

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Abstract :-

The photovoltaic effect is the direct conversion of light into electricity in solar cell .When solar cells are exposed to sunlight, electrons excite from the valance band to the conduction band creating charged particles electrons and holes. Solar cells will generate less power when exposed to high temperature compared to when they are in a cooler climate. Solar panels can often generate more electricity on a day with a cool wind and hazy sun than when the sun is blazing and temperature is high. An effort has been create to make an equation with the given data for different climate conditions of particular location Bhilwara, which is helpful to generate an equation of efficiency of photovoltaic modules with the environmental parameters like temperature, wind velocity. Here performance of module ¼ mono crystalline and multi crystalline) gives a view of impact of environmental and climatic variables and help us to find out the efficiency of modules by knowing the climatic condition of particular area.

Key words :- Ambient temperature, Wind velocity, Efficiency of solar photovoltaic module.

O-61

BALANITES AEGYPTIACA (LINN.) DELILE USED AS VETERINARY MEDICINE BY MEENA TRIBE OF TONK DISTRICT OF RAJASTHAN

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ABSTRACT

Ethnoveterinary medicine refers to people knowledge, skills, methods, practices and beliefs about the care of their animals (Mc Corkle, 1986). Meena is the largest tribe in the state of Rajasthan and represents about 50 percent population of tribal in the state. Tonk is located in north-eastern part of the state between 75°07' and 76°19' East longitude and 25°41' and 26°34' North latitude. The total area of the district is 7194sq.kms. An extensive field surveys in Meena dominated areas in the district of tonk were carried out to study the pattern of use, preparation and dosage administration of *Balanites aegyptiaca* for the treatment of ailments of animals. The study revealed that *Balanites aegyptiaca* are used in the treatment of skin diseases, wounds and diseases of respiratory systems in animals.

Key words: Ethnoveterinary, Meena and *Balanites aegyptiaca*

O-62

One-Pot Synthesis of Carbon Nanodots in an Organic Medium with Aggregation-Induced Emission Enhancement (AIEE): A Rationale for "Enzyme-Free" Detection of Cholesterol

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Addressing the limitations associated with thedetection of cholesterol,[1]we present a one-pot synthesis of acarbon nanodot (CD) in an organic medium (CDorg) from a novelbile acid hydrazone-based organogel. Interestingly, CDorg possessesthe aggregation-induced emission enhancement (AIEE) phenomenon, which rationally aids in the "enzyme-free" detection ofcholesterol through a fluorescence turn-on mechanism. On dilutionof the THF/water mixture of CDorg with its poor solvent (water), a9.8-fold enhancement in its photoluminescence (PL) emission iswitnessed. Such an enhancement in PL emission is credited to theoccurrence of molecular restrictions due to the formation ofnanoaggregates of CDorg, thereby initiating a radiative pathway forexciton decay. On adding cholesterol to CDorg, a similar enhancement in its PL emission was observed without the useof any cholesterol oxidase (ChOx) enzyme. The limit of detection and limit of quantification of cholesterol is found to be as lowas 1.09 and 3.64 μM, respectively. Hence, this contribution highlights the enzyme-free fluorescence turn-on detection ofcholesterol by a novel CD rationally designed to extend its applicability in an organic medium, where it is still considered a majorrestraint.[2]

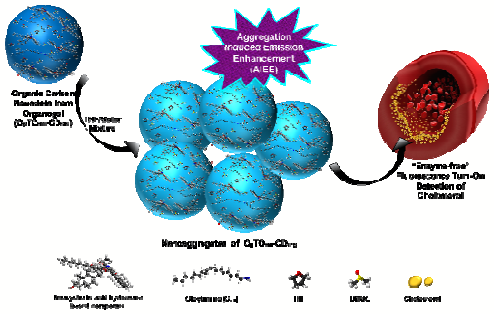

Figure: Pictorial Representation of the Formation of Nanoaggregates of Organic CDs (OgTOam-CDorg) and its Application as a Fluorescence Turn-On Sensor for Enzyme-Free Detection of Cholesterol.

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O-63

In vitro and *in vivo* antidiabetic activity of carbazole alkaloids and their pharmacokinetic study

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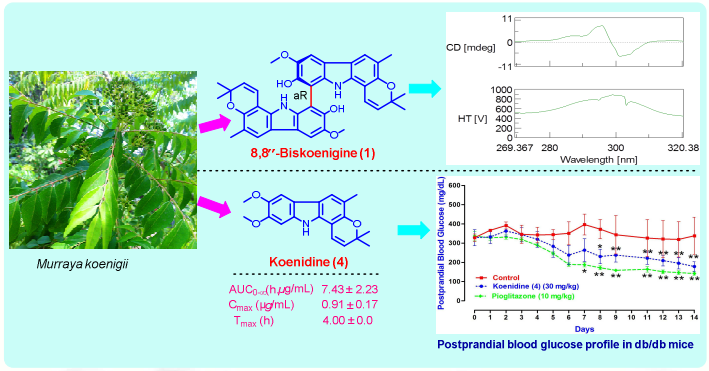
Abstract: Natural products (NPs), semi-synthetic NPs and their molecular frameworks have a long tradition in drug development and play a pivotal role in medicinal chemistry as about 49% of all small molecule drugs approved between 1981-2010.[1] Carbazole alkaloids and their derivatives are important nitrogen containing heterocycles reported to exhibit various biological activities such as antidiabetic, anti-inflammatory, antimicrobial, antioxidant, antipsychotic, anti HIV, anticonvulsant and antitumor.[2] Based on these literature reports, we prompted to isolate the carbazoles alkaloids from *Murraya koenigii* leaves to evaluate their antidiabetic activity. In this regards, we isolated carbazole alkaloids (**1**-**6**) and evaluated the antidiabetic studies.[3] After assigning the molecular structures, they were tested for *in vitro* antidiabeticactivity in L6-GLUT4*myc* myotubes. Compounds **2**−**5** showeda significant glucose uptake (under basal and insulin-stimulatedconditions) and GLUT4 translocation activity compared to rosiglitazone. The *in vivo* activity of compounds**2**−**5** in *STZ*-induced diabetic rats indicated that compounds **3**and **4** significantly decreased the blood glucose profile compared to metformin. The most significant compound,**4**, was further evaluated in leptin receptor-deficient *db/db* mice,and the mice demonstrated significantly increased insulinsensitivity and progressively lowered blood glucose level.Moreover, in vivo pharmacokinetic studies of compounds **2** and **4** clearly showed that compound **4** was 2.7 timesmore bioavailable than **2**, resulting in a superior *in vivo* efficacy. Therefore, these studies suggested that koenidine (**4**)may serve as a promising lead natural scaffold for managing insulin resistance and diabetes.



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O-64

Synthesis, Evaluation and Molecular Modelling Studies of 2-(Carbazol-3-yl)-2-oxoacetamide Analogues as a New Class of Potential Pancreatic Lipase Inhibitors

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A series of twenty-four 2-(carbazol-3-yl)-2-oxoacetamide analogues were synthesized, characterized and evaluated for their pancreatic lipase inhibitory activities. Porcine pancreatic lipase was used against 4-nitrophenyl butyrate as substrate during the inhibition assay. Compounds **7e**, **7f** and **7p** exhibited potential lipase inhibitory activity (IC50 values of 6.31, 8.72 and 9.58 µM, respectively). Further, inhibition kinetics of **7e**, **7f** and **7p** against pancreatic lipase revealed their competitive nature of inhibition. Molecular docking studies of the compounds **7a-x** into the active site of Human pancreatic lipase (PDB ID: 1LPB) was in correlation with the *in vitro* results, and highlighted probable covalent bond formation with Ser 152 apart from hydrophobic interactions with the lid domain. Molecular Dynamics simulation of **7e** complexed with PL, further confirmed the role of aromatic groups in stabilising the ligand (RMSD ≤ 4 Å). The present study led to the identification of 2-(carbazol-3-yl)-2-oxoacetamide analogues **7a-x** as a new class of potential pancreatic lipase inhibitors.

KEYWORDS: Carbazolyl oxoacetamides, Inhibition kinetics, Molecular dynamics, Orlistat, Pancreatic lipase.

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POSTERS

P-1

Design, synthesis and evaluation of 1-(4-phenylpiperazin-1-yl)ethanone based compounds as HIV-1 RT inhibitors

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Non-Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) acting upon Reverse Transcriptase (RT) enzyme of HIV-1, is an important class of antiretroviral drugs (1). In the present study, using molecular hybridization approach, thirteen (**F1-F13)** novel 1-(4-phenylpiperazin-1-yl)ethanone based hybrid compounds (Fig. **1**) were designed as HIV-1 RT inhibitor, while considering their drug-likeness behavior (2,3). Designed compounds were synthesized, characterized and *in-vitro* evaluated for HIV-1 RT inhibitory activity against wild strain, in which compounds **F1, F4, F11, F12** and **F13** displayed significant potency with $IC_{50} \leq 10$ µg/ml (4). Moreover, best active compounds of the series, **F11** and **F13** inhibited the activity of RT with IC_{50} values 6.58 and 5.97 µg/ml respectively. Structure Activity Relationship (SAR) studies were performed in order to elaborate the influence of substitution on the RT inhibitory potency. Antiviral and cytotoxicity studies of significantly active compounds (**F1, F4, F11, F12** and **F13**) revealed that except **F4,** other compounds retained significant anti-HIV-1 potency ($EC_{50} \leq 10$ µg/ml) with good safety index (5). Docking studies were performed, in order to predict the putative binding mode of the best active compound (**F13**) with wild HIV-1 RT (6).

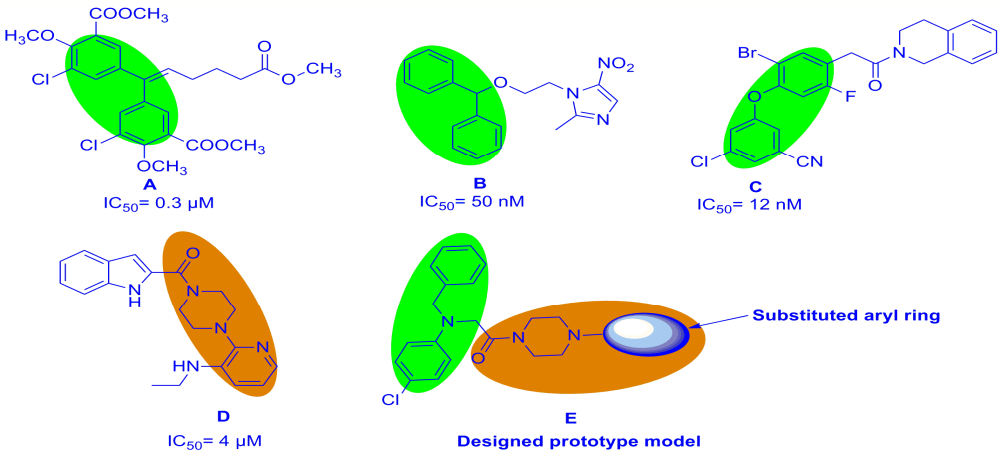

Fig. 1: Literature reported HIV-1 RT inhibitors (**A-D**) and designed prototype model (**E**)

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P-2

Development and Standardization of Polyherbal Anti-obesity Formulation(AS-22) and it's*in vitro* evaluation

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Obesity is one of the most common health problems and has become an epidemic on the global scale. In the present study, polyherbal anti-obesity formulations (AS-22) was developed and standardized as per WHO guideline [1].Anti-obesity formulation (AS-22) was developed using extracts of Triphala, Trikatu, Motha, Guggul and Vrikshamla. The developed formulation was standardized physico-chemically as per WHO guidelines and tannin, gallicacid, HCA content was estimated. *In vitro* antioxidant activity was analyzed by DPPH scavenging assay and anti-obesity activity by Pancreatic Lipase Inhibitory Activity.Physico-chemically; total ash content,acid insoluble ash,alcohol and water soluble extractive was found to be 5.23±0.25%, 1.70±0.02%, 15.93±0.55% and 35.76±0.65% respectively. LOD andBulk density was 3.01±0.14% & 0.77±0.09 g/ml. Heavy metal was not detected. Microbial load for AS-22 was found to be within the limits. Phytochemically 70.21±0.21% of tannin, 42 mg/g and 20 mg/g of gallic acid and HCA was found to be present in the formulation. AS-22 inhibited78.21±0.41% of DPPH radical with IC_{50} value 38.43±1.41 µg/ml whereas it inhibited the enzyme activities in a dose-dependent way against pancreatic lipase assay with inhibition of lipase by AS-22 (IC_{50} value10.34 mg/mL).From the above study, a potential herbal formulation AS-22 has been developed and standardized against obesity and results obtained, demonstrated for the first time AS-22 as a potent source of natural inhibitor of pancreatic lipase with powerful antioxidants proprieties that might be used in the food stabilization and the prevention of obesity complications as a complementary pharmacological drug.

Keywords: Anti-obesity, Antioxidant, AS-22, WHO

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P-3

Geometrical influence of *N*-cetylpicolinium dichromates (CPDC) on the Oxidation Kinetics of Cholesterol

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Abstract

Oxidation kinetics of cholesterol using a series of N-cetylpicolinium dichromate (CPDC), a class of phase transfer oxidants in organic media. This probing was monitored under the influence of acetic acid, surfactants (cationic, anionic and non ionic type) and solvent polarity. Oxidation of cholesterol to cholest-5-en-3-one involving an unstable cyclic transition state has been proposed and the mechanism of the oxidation is examined by solvent isotope effect along with thermodynamics study. Solvent isotope effect indicates the involvement of hydrogen exchange with the medium during cholesterol oxidation. Variation of solvent polarity is found to impose a remarkable impact on the rate of oxidation: more polar reaction environment favors the oxidation by β-CPDC oxidant to a higher extent, compared to the other two isomers: α-CPDC and γ-CPDC. The position of the methyl substituent and dimerized cluster of the CPDC are the deciding parameter of tightness of the ion pair and hence the oxidizing efficacy. CPDC oxidants are capable of oxidizing cholesterol in less time period compared to other lipopathic oxidants reported earlier.

P-4

DESIGN AND SYNTHESIS OF NOVEL HLM 006474 DERIVATIVES

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Cancer is one of the major causes of death worldwide,[1] the molecular basis of this disease involves an irregular behavior of the cellular functions mediated by receptors dependent of transcriptional factors (TF).[2]

Themutations of thegeneimplicated in thebiosyntheticpathway of E2F/pRB can be found in the 90% of human cancers[3] .Theactivation of theTFs of the E2Fs familyinducestheexpresion of genesinvolved in theprogresion of cell cycle, DNA repair, apoptosis, developementandcellular diffrenciation.[4]

HLM 006474 is a syntheticquinolinol, thatinteractsby 3 hydrogenbonds to the ADN-bindingdomain (conserved in all E2Fs transcription factors), avoidingthetranscription, andactivatingthe apoptosis[5]. The overall aim of this project is the design (by *in silico* methods), synthesis and optimization of new series of original E2Fs inhibitorsbased on thescaffold of thecommercialinhibitorHLM 006474.

Importantly, sinergiebetween HLM 006474 andcommercialanticancer agents, as for examplepaclitaxel, allowing a fast andsucessfulltraitementwasalready described.[6]

The development of new series of small, drug-like molecules, designed to optimize the interactions presented between HLM 006474 andthe ADN-bindingdomain of E2Fs is proposed as the primary project objective. These compounds are designed to constitute potential anti-cancer therapeutic leads.

The main objectives of the project are:

1) To identify new analogs of HLM006474 by drug design. (Collaboration with J.D. Maréchal, Universitéautonome de Barcelone, Spain).The **PhD student will work directly with Dr J.D. Maréchal in Spain.**
2) To synthesize the new analogs previously designed with chemistry approaches. **(PhD student work, Equipe CHROME, université de Nîmes, France).**
3) To evaluate the E2F inhibition (Collaboration with Dr. JS. Annicotte, InstitutPasteurLille, France).
4) To evaluate Cancer activity of the new analogs and to understand the mechanism responsible of proliferation inhibition. (Collaboration with Dr L. Fajas, Université of Lausanne, Switzerland).

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P-5

Sustainable 'ON WATER' chemoselective synthesis of pyranodipyrazolones *via* Ag NPs decked GO composite

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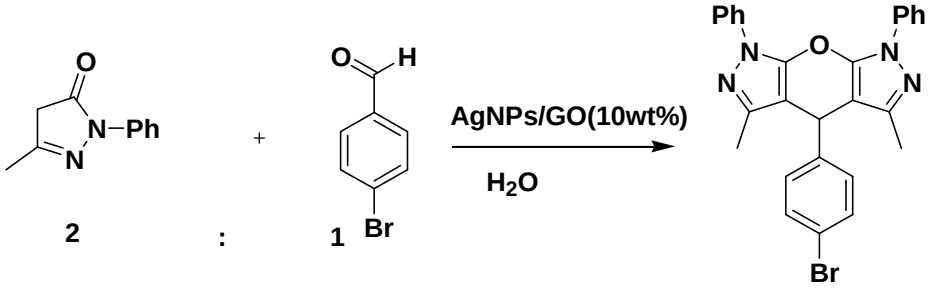
In the present scenario, growing attention is being directed towards the development of innovative catalytic systems with high performance from the point of environmentally greener processes, economical efficiency and minimum consumption of resources. Moreover the field of nanocatalysis has undergone an explosive growth during the past decade. A key objective of nanocatalysis research is to produce catalysts with 100% selectivity, extremely high activity, low energy consumption, and long lifetime. The tuning of important organic transformations and these newer generation of nanocatalysis practices worked very well together to achieve important products in sustainable way, in this regards, we have synthesized Ag NPs decked GO composite by an effective and fast one-pot chemical route incorporating the simultaneous reduction GO and preparation of Ag NPs on its surface and characterized by XRD, TEM, SEM and EDX analysis. Further we have studied its role as reusable catalyst for the 'ON WATER' chemoselective synthesis of pyranodipyrazolones *via* the reaction of different carbonyl compounds with 3-methyl-1-phenyl-*1H*-pyrazol-5(*4H*)-one. Catalyst was easily recovered by filtration and reused 7 times without any loss of catalytic activity. A highly efficient protocol has been developed for the "on water" chemoselective synthesis of structurally complex and diverse pyrano[2,3-c:6,5-c']dipyrazol]- 2-one derivatives catalyzed effectively by Ag NPs/GO composite.



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P-6

Tri-Layers Polymer Coating Enhances Biocompatibility and Activity of Drug-Loaded Magnetite Nanocarrier for Selective killing of Colorectal Cancer Cells

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Abstract: Synthetic lethal (SL) targeting of colorectal cancer cells (CRCs) using SOD1 inhibitor (LCS-1) was reported by exploiting the interaction between SOD1 and BLM. LCS-1 show poor bioavailability due to hydrophobic in nature [1, 2]. LCS-1-loaded nanocarrier (NC) of ~150 nm in size with three layers of polymers namely, aminocellulose, branched poly(amidoamine), and polyethylene glycol were prepared and characterized. Blank NC did not show any cytotoxicity towards HEK293 cells (0.5 mg/ml) mainly due to aminocellulose layer. Whereas encapsulation of LCS-1 was achieved by branched polymer layer. LCS-1-NC showed high selectivity (104 times) towards BLM-deficient over -proficient HCT116 cells and 1.7 times increased sensitivity difference for BLM-deficient cells in comparison to LCS-1 alone. LCS-1-NC induced DNA damage and apoptosis demonstrated that LCS-1-NC is very effective and specific in killing BLM-deficient CRC cells.

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P-7

Bio-inspired tetrazole tag β-carboline's: an effective prototype for the bone protection *via* inhibition of *NF-kb mediated β-catenin degradation in osteoblasts*

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Abstract: A series of novel tetrazole tag *β-carboline's* has been synthesized *via* natural product inspired molecular hybridization approach.[1] The synthetic strategy proceeds through Pre Ugi-multicomponent reaction modification. All the hybrids were examined for their bone forming potential. Three of the screened derivatives have been found to be effective in osteoblastic bone formation *in vitro*.[2] *In vitro* data strongly suggests that compound is the most promising bone anabolic agent that was therefore additionally evaluated for *in vivo* studies. Compound inhibited IKK in molecular modeling study based on docking and prevented TNFα directed IκBα phosphorylation to prevent nuclear translocation of NFκB. This prevented nuclear β-catenin degradation and promoted osteoblast differentiation.[3] *In vivo* studies show that Compound was also able to restore estrogen deficiency induced bone loss by preventing osteoblast apoptosis and promoted new bone formation increasing biomechanical strength of long bones. Histological studies on liver and uterus show that compound is nontoxic without uterine estrogenicity. Overall our results show that novel tetrazole tag *β-carboline* represents a new structural lead for bone protection Chemotherapy.[4]

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P-8

Synergistic Approach to Control Reservoir Souring in Oil Fields of Western India

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ABSTRACT:

Oilfields located in Western India produce crude oil by injection of large amounts of water. Sulfate present in injection water is converted in to sulfide by sulfate reducing bacteria. This increasing concentration of sulfide in the production fluid negatively impact oil production and known as reservoir souring [1].Biocides and metabolic inhibitors treatment can be used to control souring [2]. Biocide treatment of reservoir souring in the laboratory is studied by batch bottle bioreactor and continuous sand-packed bioreactor.

In batch bottle experiment, biocides used in this study were tetrakis (hydroxymethyl) phosphonium sulfate (THPS), benzalkonium chloride (BAC) and metabolic inhibitors were nitrate & (per)chlorate. Minimum inhibitory concentrations (MIC) of biocide THPS and BAC were 0.50mM and 0.75mM, respectively and for (per)chlorate and nitrate were 1.00mM and 1.25mM respectively. To check synergy of biocide and metabolic inhibitor $1/2^{th}$ and $1/4^{th}$ concentration of MIC was tested. Combination experiment results showed that nitrate had synergy with BAC (at $1/2^{th}$ of MIC), THPS and (per)chlorate ($1/4^{th}$ of MIC for both). Also, THPS had synergy with BAC (at $1/2^{th}$of MIC) and (per)chlorate (at $1/4^{th}$of MIC). BAC and (per)chlorate showed better inhibition at $1/4^{th}$of MIC.

The continuous sand-packed bioreactor is closely simulating the oil field condition. We successfully tested the three souring control strategies in sand-packed bioreactors; that are nitrate injection, BAC injection and combination of low nitrate and BAC. Among these treatment strategies continuous low nitrate and BAC concentration treatment showed complete inhibition of SRB activity.

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P-9

Spectroscopic Studies on the Interaction of Dye and Surface Active Ionic Liquid

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Abstract: The interaction of both cationic dye Safranine T (ST) and anionic dye Congo red (CR) with anionic and cationic surface active ionic liquid 1-butyl-3-methyl imidazolium octyl sulphate ([BMIM] [OS]) and 1-decyl-3-methyl imidazolium chloride ([DMIM] [Cl]) has been investigated by absorbance and emission spectroscopy, time resolved fluorescence study and anisotropy method at premicellar and post micellar region. The interaction of dye with both the ionic liquids occurred electrostatically as well as hydrophobically. In case of ST, initially absorbance decreases up to a certain concentration without any shift of λ_{max}, and then it increases with red shift of λ_{max}. Absorption spectra of CR gave red shifted wavelength with addition of [BMIM] [OS], but at higher concentration of surface active ionic liquid [SAIL], no shifting was observed. Again, blue shifted λ_{max} was found in lower range of [DMIM] [Cl]; but at higher concentration, it was further red shifted. Emission intensity increases in both dye-SAIL systems; for ST in both SAIL media, blue shifted spectra were observed, but there was no shift of emission maxima in case of CR in those media. Dye-IL binding ratio, binding sites and binding constants have also been calculated from fluorescence measurement. Anisotropy measurement showed that movement of dye in pre and post-micellar regions was different in different SAIL systems. Time resolved fluorescence lifetime confirmed microenvironment of dye-SAIL systems.

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P-10

An Experimental visit to study the interaction between non-steroidal anti-inflammatory drug ibuprofen and anionic surfactant AOT and effect of salt (NaI) and hydrotopes (4-4-4)

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Abstract : Ibuprofen (IBF), 2-(4-isobutylphenyl) propionic acid, is a renowned non-steroidal anti-inflammatory drug (NSAID) which is surface active and contrary to normal surfactants, having high critical micelle concentration (cmc) and hence a wider molar concentration interval of interest for the buildup of the interaction. Analyzing amphiphilic drug mixture IBF-AOT (sodium octyl sulfo succinate) tensiometric, fluorimetric, and calorimetric measurements were performed on mixed system. Presence of electrolyte and their variation of concentration at body membrane is observed which has an effect on association of amphiphilic drug, surfactant and drug-surfactant mixed system. Therefore study of mixed amphiphilic system has been done in presence of NaI which is also found at body membrane. 4-4-4 is treated here as a cationic hydrotopes as it has an ability to enhance the solubility of organic compound in aqueous medium by changing the solution properties such as viscosity, conductivity, surface tension. The steadiness of colloidal particles is intent on by a ζ-potential value, which is a measure of its surface charge and is determined with the help of dynamic light scattering (DLS) study. Comparative study of self assembly is presented comparing Clint model and experimental cmc value. Different theoretical treatments have been used to explain the molecular interactions in mixed micelles of binary combinations. Interfacial properties, thermodynamic properties are discoursed. The micellar aggregation number (N_{agg}) and micropolarity of single and mixed surfactant solutions were determined by steady-state fluorescence measurements and anisotropy (r) was measured to further shed light on the structural change at different proportion of IBF-AOT mixed micelle system. The time-resolved fluorescence profiles of DPH on DPH−AOT, DPH-IBF, DPH-IBF/AOT mixed micelle were recorded. Density functional theory (DFT) calculations showed the interaction energy comparison among all the binary, ternary and quaternary combinations.

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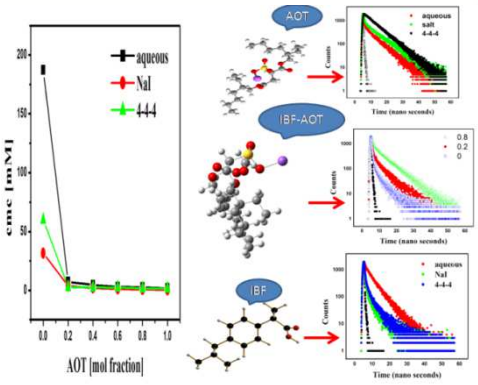

P-11

Anticancer potential of some synthesized pyrimidine derivatives

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Abstract: In 2015, about 90.5 million people had cancer. Diet, physical inactivity and obesity are related to up to 30–35% of cancer deaths. Cancer prevention is defined as active measures to decrease cancer risk. Chemotherapy is the treatment of cancer with one or more cytotoxic anti-neoplastic drugs (chemotherapeutic agents. The pyrimidine ring system has wide occurrence in nature as substituted and ring fused compounds and derivatives. The literature survey indicated that various analogs of pyrimidines have been found to possess antibacterial, antifungal, anti-inflammatory, antihypertensive, antiviral, antidiabetic, antioxidant, anticancer and calcium channel blockers. Now a day there is a great interest in synthesis and characterization of Chalcone ligands (Robinson *et al.*, 2005).

A number of substituted pyrimidine derivatives (5a-5f) were synthesized from the various substituted chalcone moieties. The structures of the compounds have been confirmed by NMR and IR spectroscopy. The in-vivo anticancer study of the synthesized compounds was investigated in swiss albino mice against 5- Fluorouracil. The anticancer activity of the synthesized compounds was done on the basis of change in haematological parameters (RBC, WBC, Hb), percentage of tumour weight inhibition (%TWI), percentage of tumour cell count inhibition (%TCI), change in body weight. The compounds showed significant activity to retard cancer cell growth (Singh *et al.*, 2010).

The result of the investigation encourages us to develop analogues and test them against various cancer models to develop more potent drugs which will act more specifically.

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P-12

Design, synthesis and characterization of hybrid urea/thiourea derivatives as a potentianl antidiabetic

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Abstract: Type 2 diabetes mellitus (T2DM) presents a major challenge to healthcare system around the world. The prevalence of diabetes is rising all over the world due to population growth, aging and urbanisation. Urea and thiourea derivatives possess many promising biological activities such as antifungal, anticancer, antimicrobial, anticonvulsant etc (Venkatachalam *et al.*, 2004).

Urea/thiourea derivatives have been synthesized and screened for the antidiabetic activity. The synthesized compounds (5a-5h) were characterized by FT-IR, NMR, Mass spectroscopy and evaluated for their both *in vitro* and *in vivo* antidiabetic activity (Dominguez *et al.*, 2005). The *in vitro* antidiabetic activity was done by α-glucosidase inhibitory activity of synthesized compounds. The *in vivo* antidiabetic activity was performed on streptozotocin induced diabetic Swiss albino rats. The Blood glucose level, different enzymatic studies (SGPT, SGOT, ALT) and lipid profile of the studied animal were estimated (Hosseinzadeh *et al.*, 2013).

The results indicated that among the series, compound 5d showed potent α-glucosidase inhibitory activity which is supported by *in vivo* antidiabetic study.

It may be concluded that hybrid urea/thiourea derivatives will be a new class of antidiabetic compound in future.

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P-13

Synthesis and characterization of Nickel(II) Complexes with 1,3-Dimethyl-5-(arylazo)-6-aminouracil

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Uracil is an important constituent of RNA, is a naturally occurring pyrimidine analogue and has numerous applications in pharmaceutical and biological sciences[1,2]. In particular, 5-aminouracil has been reported to act as an antitumoral, antibacterial and antiviral drug[3,4]. Pyrimidine dyes of 6-aminouracils have found industrial applications in hypnotic drugs,[5]living cells, detecting cancer[6]and pharmacological activities Here in we report the synthesis and characterization of metal complex of 1,3 dimethyl 6 amino uracil.The single crystal X-ray study indicates the complex adopt a square planer geometry with space group $P2_1/c$.A large number of weak intra- and intermolecular contacts are suggested in the crystal packing. Complex undergoes hdrogen bonding with the solvent molecules can be identified from NMR spectroscopy.the TD-DFT calculations was carried out for determining the electronic origin of the absorbtion spectra.

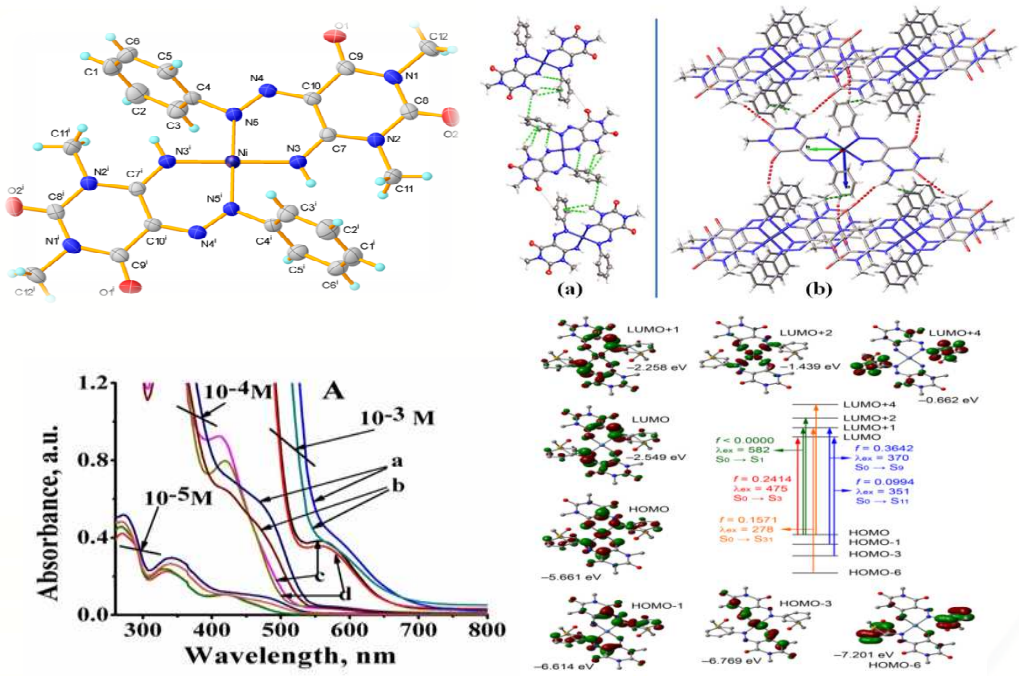

Fig. Solid and solution state characterization technique of the prepared complex

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P-14

Structure directing role of amines and water molecules in the self-assembly of polyoxomolybdates

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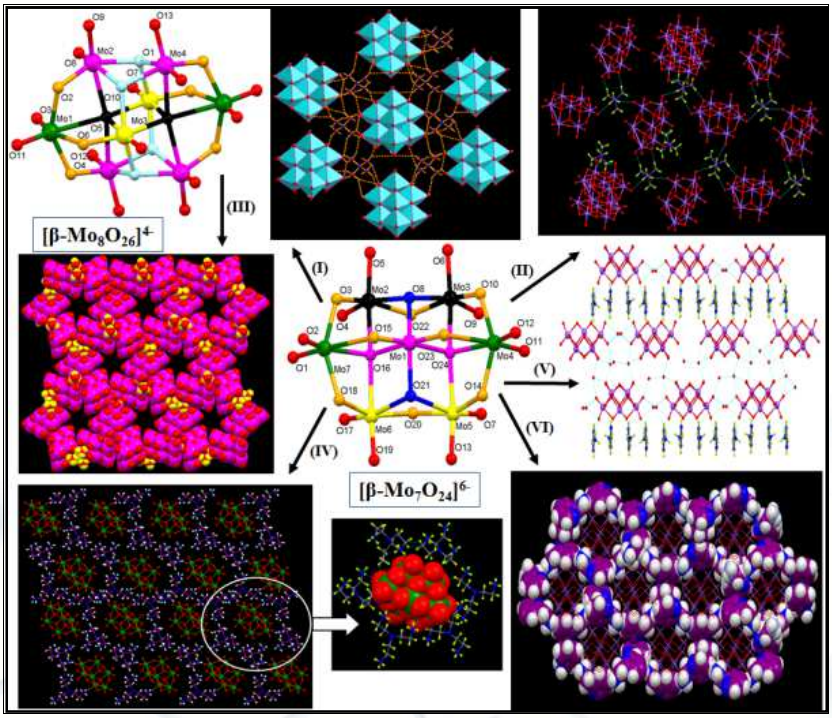
Six supramolecular complexes of charged aliphatic/aromatic amines and POM cluster anions (β-$Mo_7O_{24}^{6-}$ and β-$Mo_8O_{26}^{4-}$) are reported in an effort to study the '*Shrink wrapping*' effect of these amines on the formation of small sized unsymmetrical polyoxomoybdates (POMos). The single crystal X-ray diffraction structures of complexes **I-II (**with tetramethylammonium (TMA^+)), **III** (with tetraethylammonium (TEA^+)), **IV** (with tris(2-aminoethyl)ammonium ($TREN^{3+}$)), **V** (with 3-aminopyridinium (AP^+)), and **VI** (with 2-aminomethylpyridinium (AMP^+)) as cations, show that water, amine based cations and small size (POMo) anions are assembled to form various supramolecular architectures running from infinite 1D chains to 3D networks. Unique and interesting water clusters having W_8 to W_{21} members are formed, having 3, 4, 6 and up to 11 neighboring H-bonded water molecules in them. Steric shielding and/or "*Shrink-wrapping*" effect of organic cations is neither according to the number of amine···POMo interactions nor as their ability to wrap around the POMo. Therefore the effect has been analyzed by considering an accumulative outcome of the water clusters and the amines. Various water clusters help to envelop the POMos very effectively to prevent anion···anion interactions, helping them 'shrinked wrapped' to smaller β-$Mo_7O_{24}^{6-}$ species in complexes **I-II** and **IV-VI**. Complex **III** however, has only one water molecule, encapsulation by water is minimal and it results in the highest number of anion···anion interactions and yields bigger β-$Mo_8O_{26}^{4-}$ species. The crystallographic results have been amply supplemented by Hirshfeld surface analysis and other solid state studies.



P-15

Microwave Assisted Efficient Suzuki-Miyaura Cross-Coupling Reactions in Water Catalyzed by Nano-Pd/gC_3N_4 Composite

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The palladium-catalyzed cross coupling reactions such as Suzuki-Miyuara, Sonogashira and Heck coupling have recently gained attractiveness among the scientific community for different drug-discovery and development programs. Especially, Suzuki-Miyuara cross coupling reaction is most critical reaction has found to important building blocks used in the creation of a broad range of biaryls, including natural products, pharmaceuticals and advanced materials (1). Due to broad applications of Suzuki-Miyuara cross-coupling reaction, development and design of better catalysts have been attracted the attention of scientific community. homogeneous Pd-catalysts have some serious drawbacks such as contamination of metal in the products, difficulty in isolation of soluble metal-complexes and no recyclability makes their application less attractive and cumbersome for industrial use (2). Therefore heterogeneous supported catalysts have been received a powerful attention for C-C bond formation. The significance of heterogeneous catalysts are facile separation of metal-catalysts, reusability and environmental benign. In recent past, palladium NPs have been utilized as the most efficient catalyst to C−C bond formation reactions like Suzuki−Miyaura coupling reactions in term of the economic benefits, large surface area and high catalytic activity (3). Pd NPs on the surface of supports, such as microporous polymers, nano-silica, or carbon materials. But aggregation and leaching of the nanoparticles creates problems. Graphitic carbon nitride (g-C_3N_4) exhibit attractive properties such as chemical stability, thermal stability, water resistance, low density and two layered structure presents itself as one of the most suitable material to disperse Palladium nanoparticles (4). On other hand water is most considered as an environmentally benign solvent because of it is cheap, non-toxic, and readily available. Herein we report the high efficiency Suzuki-Miyaura cross coupling reactions using nanosized palladium catalyst supported on graphitic carbon nitride (nano-Pd/gC3N4) in water as solvent and using microwave irradiation as a green methodology towards development of sustainable catalytic process for biaryls. Details about optimization of reaction conditions and synthesized various darivatives will be discussed during presentation in conference.

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P-16

Chemo–, Regio– and Stereoselective *N*–alkenylation of Pyrazoles/Benzpyrazoles using Activated and Unactivated Alkynes

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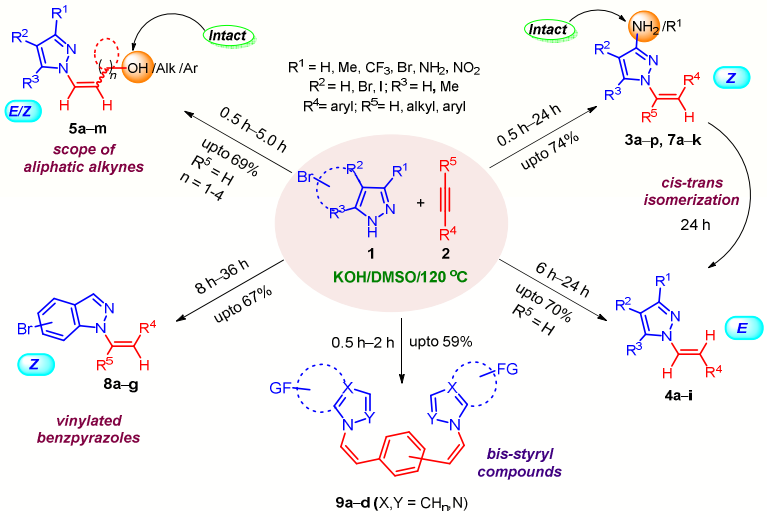

Transition–metal–free chemo–, regio– and stereoselective synthesis of (*Z*) and (*E*) styryl pyrazoles and benzpyrazoles by the addition of *N*–heterocycles onto functionalized terminal and internal alkynes using a super basic solution of KOH/DMSO has been described. The stereochemical outcome of the reaction was governed by time and quantity of the base. The reaction of pyrazoles and benzpyrazoles onto alkynes takes place chemoselectively without affecting the free –NH_2 group of pyrazoles and –OH group of alkynes. This developed methodology also provides easy access for the synthesis of bis–vinylated heterocycles. For the first time, we have disclosed the base-mediated conversion of (*Z*)-styryl pyrazoles to (*E*) styryl pyrazoles in KOH/DMSO system. The cis–trans isomerization was supported by the control experiments and deuterium labeling studies.

Acknowledgements
The work was supported by DST and University of Delhi. V. G. is thankful to CSIR for fellowship.
Institution/ person name
University of Delhi, c/o Prof. Akhilesh K. Verma.

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P-17

Non-peptidic Glucagon-Like Peptide-1 Receptor Agonists for Anti-diabetic Therapeutics

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The dual epidemics of obesity and Type 2 diabetes (T2DM) represent an enormous challenge to our health care system. Glucagon-like peptide-1 (GLP-1) receptor (GLP-1R) agonists have emerged as treatment options for T2DM. A naturally occurring GLP-1R agonist, exendin-4 (Ex-4), is now available for treatment [1]. However, due its peptide nature, Ex-4 is only administer through injection [2] and furthermore, evidences mainly collected from animal models, have indicated the role of GLP-1 in increasing beta-cell proliferation and differentiation and in decreasing the rate of beta-cell apoptosis can leads to pancreatitis and cancer [3]. Therefore, there is a need to search for small molecules which can mimic GLP-1R agonists with increased efficacy lesser and side effects to overcome the pitfall of present day GLP-1R's peptidic agonists. Here we report the discovery of the potent and selective GLP-1R agonist, PK2. We identified PK2 in a low throughput cAMP inducer-based screening of large combinatorial small molecules library, and show that PK2 promotes G-protein signalling comparable to Ex-4. This non-peptide compound, PK2, binds with micromolar affinity to the human GLP-1R and induced cAMP production and GLP-1R internalization. In vitro studies using different cell lines demonstrate that PK2 treatment protected liver cells from palmitate induced lipotoxicity. PK2 attenuates palmitate induced endogenous lipogenesis through suppressing the promoter activity of fatty acid synthase. Nevertheless, PK2 rescue liver cells from chronic hyperinsulinemia induced insulin resistance, suggesting that PK2 may provide a novel therapeutic approach to T2DM.

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P-18

New Derivatives of Substituted Amino Uracil: Synthesis & Its studies on Aerobic and Anaerobic (Hypoxic) Mycobacterium Tuberculosis.

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ABSTRACT: Tuberculosis is fast emerging as a threat and a cause of global concern that needs both surveillance and control. Drug therapy is the cornerstone of TB management[1]. However, the prolonged duration of the current therapy, the non-compliance of patients, the occurrence of multidrug-resistant(MDR) and extensively drug-resistant(XDR) and any one of strains along with the increased co-incidence of HIV cases[2], high relapse rates and latent infection have all made the effective control and management of the disease difficult. Dormancy is a major reason for prolong 10-12 months duration of TB treatment and clearing of bacterium *M. Tuberculosis*. Dormancy also causes the lifelong reoccurrence of the disease[3]. A modified method was optimised for synthesis of substituted amino uracil schiff bases. Various compounds were synthesized and Characterization was done .Physicochemical properties of synthesized compounds were determined insilico. Compounds were tested in hypoxia induced dormancy model in Mycobacterium bovis BCG strain (vacutainer model). Hypoxic culture (21 days old) were incubated for next 10 days with synthesized amino uracil schiffs bases, standard antibiotics and vector controls. Isoniazid is used as negative control, Metronidazole as positive control and 5% DMSO were used as vector control (did not inhibited the growth of anoxic culture). A novel scaffold Compound E has shown promising inhibition (63%) at the concentration of 250 µM. Compound E is identified as potential hit against dormant Mycobacterium.

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P-19

Syntheses, crystal structure and solid state properties of lanthanoid containing nanocluster: $[(Ln_2SiW_{10}O_{38})_4(W_3O_8)(OH)_4(H_2O)_2]^{26-}$

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Polyoxometalates (POMs) are eminent category of inorganic metal-oxygen clusters in which early transition metals of group V and VI (mostly Mo(VI), W(VI) and V(V)) are in their high oxidation state, having an unrepeatable structural variety combined with a superfluity of properties[(1)]. POMs are not only remarkable in the sense of molecular structure changeability, but also due to their reactivity and potential application in several fields such as biology, medicine, material science, catalysis[(2)], magnetism[(3)], clinical chemistry, photochemistry, and analytical chemistry. Lacunary POMs with empty sites on addendum metal positions are much more reactive to act as wonderful inorganic multidentate O-donor ligands towards elctrophiles. Due to highly negative charge surface they can coordinate with transition metal (TM) or rare-earth (RE) cations to construct pleasant architectures. Consequently a multitude number of TM-, RE-, or RE-TM- substituted POMs have been prepared so far[(4)]. A series of lanthanoid-containing polyoxometalates have been synthesized by the reaction of $Na_{10}[\alpha\text{-}SiW_9O_{34}].16H_2O$ with $Ln(NO_3)_3.nH_2O$ by using one step self-assembly process in potassium chloride solution. The reaction of $Na_{10}[\alpha\text{-}SiW_9O_{34}].16H_2O$ with $Ln(NO_3)_3.nH_2O$ leads to the formation of the tetrameric silicotungstate $[(Ln_2SiW_{10}O_{38})_4(W_3O_8)(OH)_4(H_2O)_2]^{26-}$ [Ln =Sm^{3+} (**a**), Eu^{3+} (**b**), Gd^{3+} (**c**), Tb^{3+} (**d**), Dy^{3+} (**e**), Ho^{3+} (**f**), Er^{3+} (**g**), Tm^{3+} (**h**), Yb^{3+} (**i**), Y(**j**)]. Most of the title compounds were analysed by various analytical techniques such as FTIR, UV/Vis, and photoluminescence, TGA/DTA.

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P-20

Molecular and chemical fingerprinting tools for the identification of adulterants in Saffron

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Saffron (*Crocus sativus* L.),the most expensive spice, is used worldwide for its flavor, color and medicinal properties. Owing to its high economic value and restricted production, it is often subjected to adulteration. The international and national standards available are mainly helpful in finding the dyes present and to detect the presence of non-saffron substance by taxonomic methods[1] butit is important to find the adulterants present in the commercial sample as some of them have been reported to be toxic to humans[2]. Methods like HPLC and HPTLC are effective in finding the chemical adulterants presentbut they fail to find the plant adulterants, whereas, DNA barcoding is effective in finding the plant adulterant but not the part of the plant. So, in our study we have used HPLC, HPTLC and DNA barcoding to authenticate the market sample and to detect the adulterants. Authentic saffron was collected from Pampore valley, Kashmir. The HPLC fingerprint, HPTLC fingerprint and the authentic DNA barcodes were obtained. Market samples were collected from India and abroad. The HPLC, HPTLC and DNA barcoding analysis of market samples were standardized and the results obtained were compared. The results reported a large number of new adulterants and the combinatorial method of molecular and chemical fingerprinting was found to be effective in authentication and identification of adulterants in saffron. This method can also be used as a method for quality control of commercial saffron.

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P-21

Metal-free regioselective tandem synthesis of functionalized benzimidazo-fused benzofuro[3,2-*c*]pyridines, γ-carbolines and benzofuro/thieno[2,3-c]pyridines in aqueous medium

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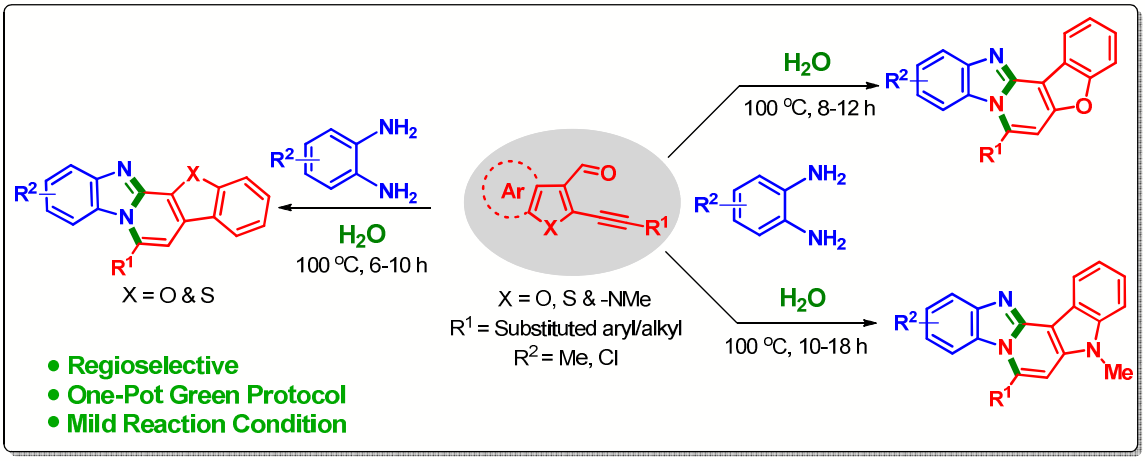
In the continuation of our ongoing lab work using *ortho*-alkynyl aldehydes,[1,2] we have design an operationally simple greener approach for the synthesis of broad range of functionalized benzimidazolo-fused benzofuro[3,2-*c*]pyridines, benzofuro/thieno[2,3-*c*]pyridines and γ-carbolines under the metal-free condition in water has been described. The aqueous medium accelerates the formation of desired product by avoiding side-product as well as drastic reaction condition. The reaction proceed through inter and intramoleculer C-N bond formation in one-pot *via* 6-*endo*-*dig* cyclization. The deuterium labelling and X-ray crystallographic studies supported the proposed mechanistic pathway for the targeted cyclized product.



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P-22

Preparation and characterization of alveolar macrophage targeted drug delivery system for hydrophilic drug

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Alveolar macrophages are the pivotal regulators of immunological homeostasis and key effector cells in the first line host defense[1]. This mechanisn is blocked upon infection with some bacterial infection and the alveolar macrophage cells start serving as sanctuary for the lodging and growth of various bacteria. Chitosan, a biocompatible polymer, is hydrophilic and soluble in acidic solvents, and thus it is easy to encapsulate hydrophilic drugs[2]. In addition, due to its mucoadhesive properties, it also has antioxidant property[3]. In the present research work we use antioxidant property of chitosan and ascorbic acid to treat mycobacterial infection. We formulate here chitosan based alveolar targeted drug delivery system for isoniazid. This synergistic antioxidant activity of both could be use for alveolar macrophage and lung targeting of various drugs.

Keywords: Chitosan, Alveolar Macrophage Targeting, Antioxidant property

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P-23

Nonlinear Effects at Soft Interface of an Emulsion in List-Lerner-Barbas Aldol Reaction Catalyzed by Surfactant Based Proline Catalyst

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The observed homochirality in the living world has fascinated chemists for centuries. Nonlinear effects in asymmetric synthesis enhance our understanding towards origin of chirality.[1] Since the first report on nonlinear asymmetric induction by Kagan et.al.,[2] it has been investigated critically for several other chemical reactions including List-Lerner-Barbas aldol (LLB-A) reactions.[3] Several theories like dissolution-crystallization [4], aggregation,[5] and phase transitions of catalysts[6] have been considered to explain the observed non linearity in asymmetric organocatalyzed aldol reactions.

In the series of extending LLB-A reactions in aqueous media, synthetic methodologies with modified proline surfactant catalysts have been developed. In the present report, a model LLB-A reaction proceeding in emulsifying condition, catalyzed by amphiphillic proline-based catalyst has been investigated. Scalemic mixtures of catalysts were used and interesting deviation from linear behavior was observed. In order to explore interfacial chirality Congo Red was employed as achiral probe. The non linearity was also reflected in the CD responses of amphiphillic catalyst- Congo Red heteroaggregate. The observations were interpreted in terms of catalyst equilibration and phase behaviour of two enantiomers of catalyst in emulsifying conditions. [7]

This is the first report of nonlinear behaviour for aldol reaction at soft interface of a surfactant aggregate.

Further investigations hold promising potential to understand the origin of chirality.

Scheme1. Model LLB-A reaction of cyclohexanone and *p*-nitrobenzaldehyde in presence of amphiphillic catalyst.

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P-24

Invitro release study of Camptothecin from functionalized Mesoporous silica materials

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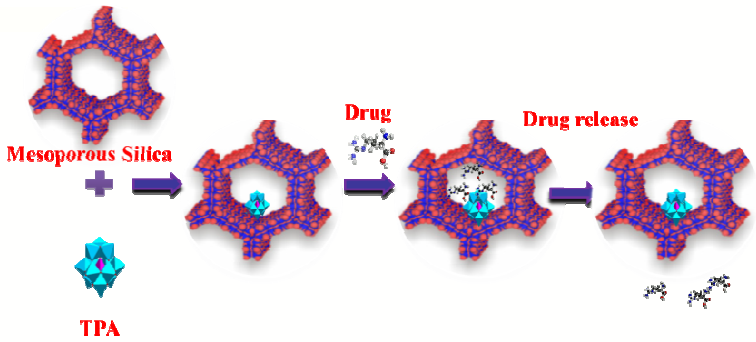
Abstract

Camptothecin (CPT) is a naturally occurring quinolone alkaloid which shows significant anticancer activity with a broad spectrum of human malignancies and CPT is an inhibitor of the DNA-replicating enzyme topoisomerase-I. Unfortunately, the clinical application of CPT is hindered by its poor pharmaceutical profile, with extreme aqueous insolubility, low stability of the lactone form at physiological pH, and severe systemic toxicities which included myelosuppression, vomiting, diarrhoea, and hemorrhagic cystitis. The mentioned problem can be overcome by using proper delivery systems. Mesoporous silica materials have gained much attraction in the field of drug delivery as they have several attractive features for controlled release. To control the release rate of drug, these mesoporous silica materials have been functionalized by various organic groups.The present paper deals with the functionalization of MCM-41 and MCM-48 using 12-tungstophosphoric acid (TPA). TPA-MCM-41 and TPA- MCM-48 have been selected to study the controlled release of Camptothecin.



In present paper, the synthesis, functionalization of mesoporous silica (TPA-MCM-41 and TPA-MCM-48), encapsulation of Camptothecin and their characterization using variousphysicochemical techniques as well as cytotoxic study will be described. MTT study was carried out using Human hepatocellular liver carcinoma (HepG2) cells. In vitro controlled release of Camptothecin was carried out in simulated body fluid, at body temperature, under stirring as well as static condition. Investigation of release kinetic and mechanism was also carried out using first order release kinetic model and Higuchi model.

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P-25

Active Targeted Thymol Encapusulated *In-Situ* Synthesized Bimetallic (Au/Ag) Nanoparticles Containing Nanogels as High Efficiency Anti-Cancer Agent

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ABSTRACT: The use of nanotechnology in cancer treatment offers rousing possibilities, including the leeway of destroying cancer lumps with minimal mutilation to healthy tissue and organs. Here, in our work polymer based nanogels formulations by using amine modified guar gum (Agg) offers *in-situ* synthesis of pure monometallic silver (Ag) and gold (Au) and bimetallic Au/Ag nanoparticles. The morphology and structure of the nanoparticles were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and energy dispersive X-ray spectroscopy (EDX), which confirmed the formation of spherical mono and bimetallic nanoparticles. UV-vis absorbance spectroscopy and TEM results indicated that both size and optical properties of the Ag, Au and Au/Ag nanoparticles in the Agg can be controlled vis-a-viz Agg polymer concentration and ion content. Thymol, an herbal monoterpene phenol act as biocidal and anticancer agent was loaded into mono and bimetallic assisted nanogels. Thymol loaded metal assisted nanogels showed slow and sustained release profile at cytosolic pH. Furthermore, we address key biological aspects of synthesized mono and bimetallic assisted nanogels for targeting drug carrier design in skin cancer cells (Kera-308). Folic acid (FA) has been used to recognized cancer cells and coupled with Agg. Cell viability data showed preferential ameliorated cytotoxicity of bimetallic Au/Ag in construct to mono metallic Ag, Au nanoparticles. Thymol encapsulated Au/Ag nanogels showed significant elevation in production of reactive oxygen species (ROS) activity and depolarization of mitochondrial membrane potential. The study illustrated that FA conjugated thymol loaded Au/Ag bimetallic nanogels is admirable non-invasive therapeutic agent against skin cancer.

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P-26

Diversity oriented synthesis of β-carbolinone and indolo-pyrazinone analogues based on an Ugi four component reaction and subsequent cyclisation of the resulting indole intermediate

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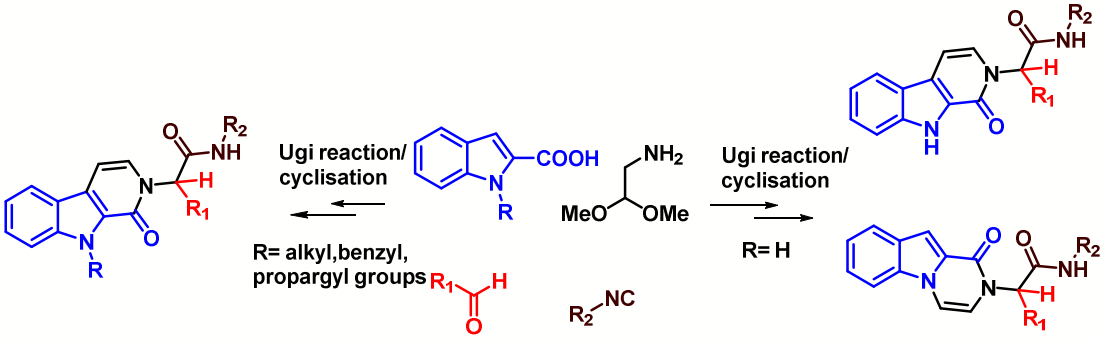
Abstract: The Ugi-4CR offers a powerful and atom-economical way to construct functionalized molecular architectures from readily available starting materials. The combination of multicomponent reactions with post-condensation modifications has proven to be a powerful tool for accessing novel heterocyclic scaffolds.(1)Indole heterocyclic, β-carboline core containing natural products and related synthetic derivatives have found extensive application in medicinal chemistry.(2) Moreover, pyrazinones derivatives are found alone and/or embedded with several privilege heterocyclics which displays prominent biological activity and are featured in several naturally occurring molecules and synthetic derivatives.(3)

In the light of above fact, herein we report an efficient one-pot domino multicomponent reaction for the synthesis of highly functionalized β-carbolinones and indolo-pyrazinones. The reaction involves an Ugi-four component reaction followed by *in situ* acid mediated deprotection/activation/electrophilic cyclisation/and aromatisation. The potential of this methodology is proved by development of a diverse library of heterocyclic compounds with point and skeletal diversity.



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P-27

One-by-one Imprinting in two Eccentric layers of Hollow Core-shells: Sequential Electro-analysis of anti-HIV drugs

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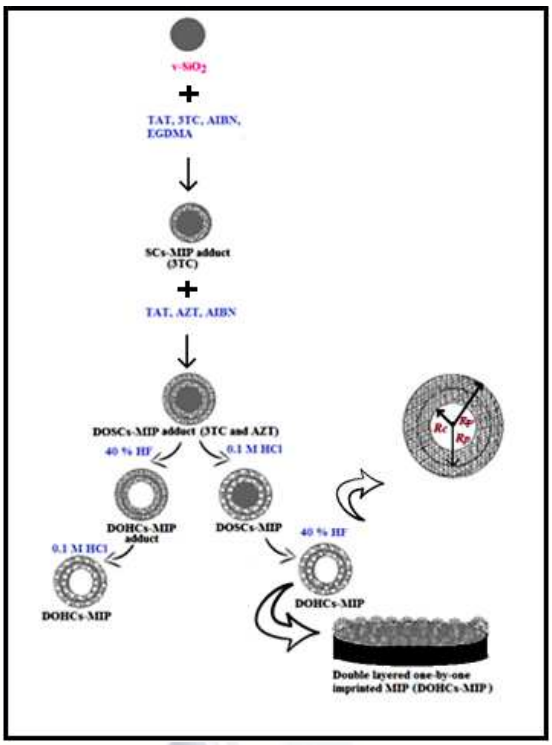
ABSTRACT: Double layered one-by-one imprinted hollow core-shells@ pencil graphite electrode was fabricated for sequential sensing of anti-HIV drugs. For this, two eccentric layers were developed on the surface of vinylated silica nanospheres to obtain double layered one-by-one imprinted solid core-shells, which on treatment with hydrofluoric acid yielded hollow core-shells [1]. Whereas modified hollow core-shells (single layered dual imprinted) evolved competitive diffusion of probe/analyte molecules, the corresponding double layered one-by-one imprinted hollow core-shells (outer layer imprinted with Zidovudine, and inner layer with Lamivudine) were found relatively better [2,3] owing to their bilateral diffusions into molecular cavities without any competition. Therefore, entire work in this article is based on differential pulse anodic stripping voltammetry at double layered one-by-one imprinted hollow core-shells, which imparted indirect detection of electro inactive targets with limits of detection as low as 0.91 and 0.12 (aqueous sample), 0.94 and 0.13 (blood serum), and 0.99 and 0.20 ng mL^{-1} (pharmaceutics) for lamivudine and zidovudine, respectively in anti-HIV drug combination.



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P-28

Scientific importance of XRD Analysis of Ayurvedic Bhasma

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Abstract: In Ayurvedasystem of medicine, metallicbhasmas have been found to playa very important role since thousands of years.Ayurveda uses metals and minerals in the form of bhasma (fine powder obtained through calcinations). These bhasma are useful in control of manydiseases. It is well known that many such good compositions are well prepared in ayurveda, but thereafter to prove its scientific capability, many scientific standardization techniques (XRD,DLS,ICPMS,SEM,TEM) etc. are carried on ayurvedic bhasmas, that have proved how thesebhasmas are scientifically perfect.Out of these techniques, X-ray powder diffraction (XRD) is one of the most powerful techniques for qualitative and quantitative analysis ofayurvedicbhasmas.X-ray powder diffraction is a rapid analytical technique primarily used for phase identification of a metallic bhasma and can provide information on unit cell dimensions of the molecules present in the sample. The most widespread use of powder diffraction is in the identification and characterization of crystalline solids, each of which produces a distinctive diffraction pattern nature of crystalline phase present, structural make-up of phases, degree of crystalline, amount of amorphous content, micro strain, and orientation of metallic bhasmas. Particle size is calculated from XRD by using Debye Scherer formula $D = 0.9 \lambda / \beta \cos \theta$. Thus, this technique helps us to correlate the effectiveness of any ayurvedic medicine with its particle size.

Keywords: AyurvedicBhasma, Standardization techniques, XRD,Particle size

P-29

Synthesis and evaluation of Ni/ZSM-5 for dehydration of glycerol to ethylene

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Abstract: A continuous flow fixed bed reactor is established to investigate the process for conversion of glycerol to ethylene. The glycerol is added in water with (10%, 30%, 50%) composition. The reaction temperature was set to 600°C to achieve maximum selectivity towards ethylene. However, large amount of carbon dioxide along with ethylene is also produced during the reaction. To lower the deactivation of ZSM-5 catalyst, metal incorporation over ZSM-5 was done by incipent impregnation method Wang et al [1]. The best results were obtained at 30% glycerol in water at which product selectivity and catalyst lifetime were 28.7 % and 15 hours with Ni/ZSM-5 catalyst. At high reaction time, glycerol conversion is maximum. Process variables like temperature and reaction time are also studied to demonstrate the effect on conversion, selectivity and deactivation of catalyst. Generally, the conversion rate of glycerol decrease with reaction time. The reaction products were analyzed by gas chromatography. The gas products were analyzed in Propack-Q column and liquid products were analyzed in capillary column.

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P-30

Neuromodulatory Action of Exogenous Oxytocin (OT) and Antagonist (OTA) by GABAergic Transmission in Different Region of Brain.

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Abstract: Oxytocin is a neuropeptide synthesised in hypothalamus by neurosecretory cells (magnocellular neurons) of the hypothalamic paraventricular (PVN) and supraoptic nuclei (SON), while stored and finally secreted by posterior pituitary lobe in blood circulation Bargmann, 1949 (4). In central action oxytocin act as neurotransmitter and release of oxytocin within the brain occurs from dendrites, axon and somata of magnocellular neurons of the paraventricular nucleus in different region of brain Landgraf and Neumann *et al*., 2004 (1). In peripheral action oxytocin (OT) is a hormone but in central action specific receptors are present in brain and help in neuromodulations. It has been shown that receptor distribution varied with age Tribollet *et al.*,1989 (3).and species of animal Raggenbass, et al. 1989 (2). Oxytocin (OT) affect social life in mammals and interest is growing toward neuropeptide and their region specific receptors which could be important for the designing of new drugs targeting specific neuropsychiatric disease Marta Busnelli 2013 (5). In this part of experiment synthetic oxytocin (OT) and atosiban (OTA) show alteration in GABA concentration in different region of brain as compared to control female mice, *Mus musculus.* Detail mechanism and methods will be discussed in presentation .

Keywords: Neuropeptide, neurotransmitter, receptor, Neuromodulation & Alteration

Founding and Disclosure:- This work was supported by the founding agency MPCST (Madhya Pradesh Council of Science and Technology) order no. 1676/CST/R&D/(BS)/2015.The authors declare no conflicts of interest.

Acknowledgments: We thanks Dr. Sunando Datta, Associate Professor, Department of Biological Science, Indian Institute of Science Education and Research (IISER), Bhopal for their excellence Instrument facility assistance.

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P-31

CHEMISTRY UNDERLYING THE ACTIVITY OF ORGANOSULFUR COMPOUNDS OF *Allium sativum*

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Abstract: *Allium sativum* (Garlic) is mainly rich source of organosulfur compounds. It is a bulbous natural plant belongs to the lily family, Liliaceae. Potentially active chemical constituents of *Allium sativum* are organosulfur compounds, amino acids, minerals and enzymes. Organosulfur compounds such as allicin, ajoene, diallyl sulfide (DAS), diallyl disulfide (DADS) and others are mainly responsible for the bioactive properties. The chemistry underlying the significant biological activity of *Allium sativum* is associated with the increased hydrogen sulfide signaling in the body. It is a popular herbal product due to its potential for disease prevention and treatment. Its leaves, flowers and cloves have been used for culinary and medicinal purposes from ancient times. It has multiple biological properties, such as immunomodulatory, antimicrobial, anticarcinogenic, antioxidant, antidiabetic, anti-inflammatory, nephroprotective, hepatoprotective, neuroprotective, antiplatelet, hypolipidemic and cardioprotective. This article studies the chemical mechanism behind the activity of organosulfur compounds present in *Allium sativum.*

Keywords: *Allium sativum*; Organosulphur compounds; Allicin; Ajoene.

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P-32

"Zero VOC" synthetic strategy – Aromatic Amination reactions in deep eutectic solvents

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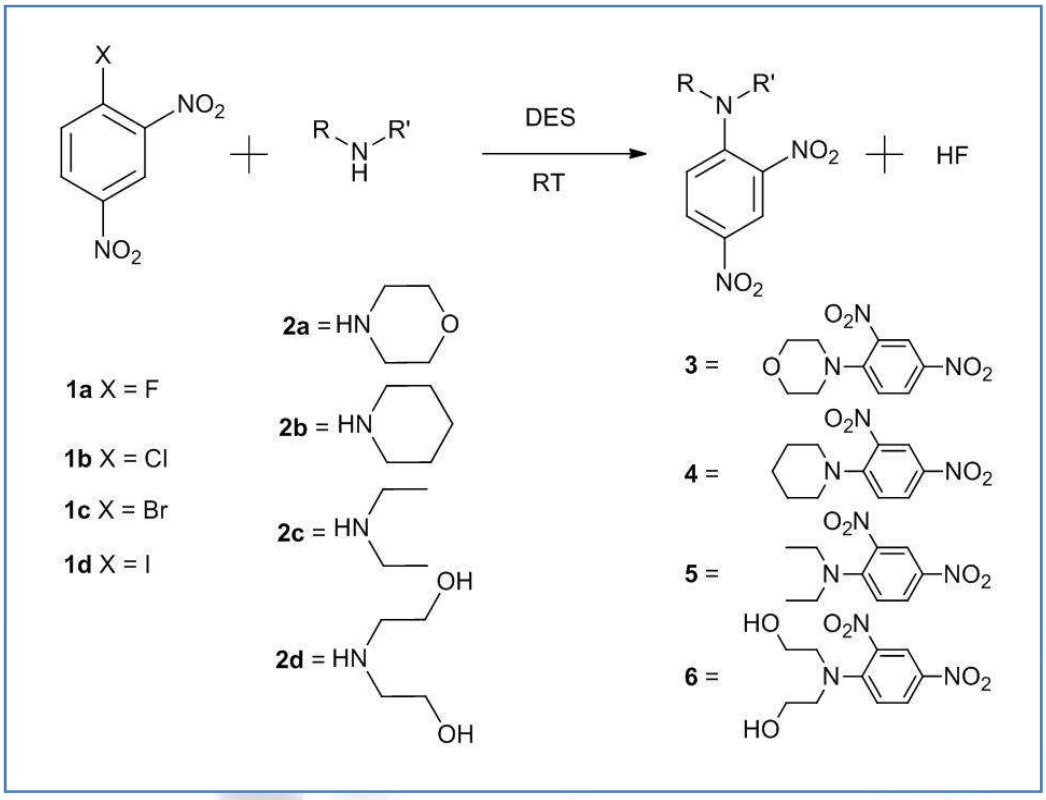
Rising concerns for environment is prompting many chemists to use "green" solvents like water, polyethylene glycol, ionic liquids and deep eutectic solvents (DES). However, barring a few instances, many of these processes still suffer from the need to use volatile organic solvents for the workup and isolation of products. In the present report, we demonsrate a "zero VOC" protocol which eliminates the need to use organic solvents for any stage of the reaction. Nucleophilic aromatic substitution reactions of with secondary amines were carried out in deep eutectic solvents to give excellent yields, as a proof of concept. The reaction workup involved the addition of water for separating the product from the DES. Evaporation of water led to recovery of the DES, which exhibited good recyclability.



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P-33

Phytochemical fingerprinting of the pods of edible legume *Cyamopsistetragonoloba*(Guar) of different regions of Rajasthan

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With the ever increasing need for finding novel drugs to combat the human diseases and to improve the quality of life, there has been extensive research going on phytochemicals and their medicinal properties. *Cyamopsistetragonoloba* (Guar)is an important legume of the desert state of Rajasthan region.The pods of this legume have been used by local people as a vegetable and also for various medicinal applications. Legumes in general are important specific sources of the medicinally valuable isoflavonoids/flavonoids. These compounds are known to have anti-cancerous, anti-inflammatory, antioxidants and other health promoting properties [Wei et.al.,1995]Though there are reports available regarding the presence of theisoflavonoids/flavonoids like daidzein and genistein in the seeds of guar [Sharma et.al.,2011] but detailed investigation regarding the region wise analysis with respect to presence of isoflavonoids/flavonoids and their glycosides is lacking for the same. The present study undertakes phytochemical fingerprinting of guar pods from six different regions of Rajasthan area. They were subjected to methanolic extraction followed by column chromatography using Amberlite XAD7-HP matrix. The elution was performed using 100% Methanol and the eluents were analyzed using High Performance Thin Layer Chromatography(HPTLC) and High Performance Liquid Chromatography(HPLC). The HPTLC and HPLC results showed that there were differences in the phytochemical profile of Guar obtained from different regions. The data obtained shall be presented in detail during the presentation.

Keywords: *Cyamopsistetragonoloba*,fingerprinting, isoflavonoids, HPTLC, HPLC.

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P-34

Synthesis and Characterization of Ionic Palladium Catalyst - $Ti_{0.97}Pd_{0.03}O_{1.97}$: Application in Suzuki - MiyauraCoupling Reaction

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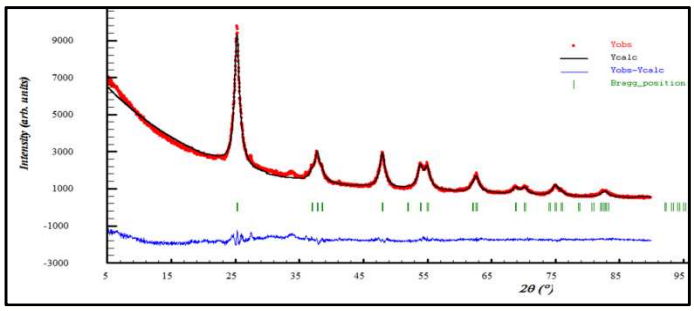
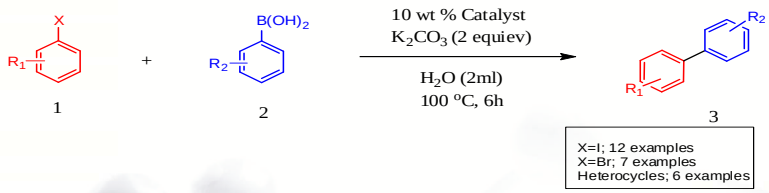
Abstract:$Ti_{0.97}Pd_{0.03}O_{1.97}$ is a nano catalyst which is prepared by the solution combustion method[1,2]. Burning the solution of stoichiometric amount of Titanyl nitrate, palladium chloride and in presence of fuel such as oxalyldihydrazide or glycinesolution, it is possible to get the ionic palladium single phase catalyst *i.e.*$Ti_{0.97}Pd_{0.03}O_{1.97}$. This is characterized using X-ray studies. Rietveld refinement analysis (Figure 1) also performed to calculate lattice parameter, h k l values and average crystal size. Using Scherrer formula and Full width at HalfMaxima method (FWHM), the calculated size of the catalyst is about 8±2 nm.By solution combustion method it is possible to coat this catalyst on cordierite honeycomb [3]. It is a ceramic material with cylindrical structure made up of many parallel channels of square shape. The composition of cordierite honeycomb is $Mg_2Al_4Si_5O_{18}$.

Figure 1: Rietveld refinement profile



Scheme 1: Suzuki - Miyaura coupling reaction



Suzuki - Miyaura coupling (SMC) reaction (Scheme 1) is a synthesis of biphenyls from arylboronic acids and aryl halides. The SMC reaction is very well known reaction with palladium catalyst. $Ti_{0.97}Pd_{0.03}O_{1.97}$is very good catalyst in the synthesis of various biphenyls. The powder catalyst is used for the SMC reaction. Some of the substrates of biphenyl are synthesized using catalyst coated cordierite honeycomb and we observed same percentage of yield in both the cases. Powder catalyzed reactions are done in a small reaction vial about 6mL capacity with a screw cap whereas cordierite honeycomb coated ionic palladium catalyzed reactions are performed in a modified reaction flask. SMC reactions are done in water as solvent at temperature of 100°C. It takes 6 hours for completion of the reaction. About 24 substrates scope have been done using powder ionic palladium catalyst and about 8 substrates are done with cordierite honeycomb. All the reaction products are characterized using ^{1}H NMR and ^{13}C NMR.The recycling of the coated catalyst have been done for same substrates

for 7 times. After 7 cycle of the reaction the percentage yield is about 4 – 5% lesser than that of first cycle.

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P-35

Genome size and Ty1 *copia* retroelements in biofuel crops

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Abstract: Non-edible oil crops like *Pongamia pinnata*, *Jatropha curcas*, *Ricinus communis* and *Mesua ferrea* are considered as a sustainable source of feedstock for biodiesel industry. Research and progress on these plants are dependent on an extensive knowledge of the genome structure. Till date, there has been no genomic research aimed at the exploring the biotechnological potential of these species. In the current study, the nuclear DNA content, was estimated with the aid of flow cytometry and the genome size (2C DNA) was in the order of *J. curcas* (0.86 pg), *R. communis* (1.01 pg), *M. ferrea* (1.4 pg) and *P. pinnata* (2.49 pg). Intra-specific variations were observed in genome size whereas no such variations in the chromosome number were detected in plants collected from different eco-geographical regions. This attributed to reverse *transcriptase-RNase H* (RT-RH) domains of Ty1-*copia* retrotransposons. Dot-blot analysis revealed that the Ty1-*copia* accounts for 2 % to 9.5% of total haploid nuclear genome for the above mentioned plants and phylogenetic analysis showed that RT-RH sequences are heterogeneous that resolved into distinct, different groups. The results contribute to preliminary understanding about genome organization and evolution.

P-36

Green Synthesis of Silver Nanoparticles Using a Wild Edible Mushroom *Termitomycesheimii* and Their Bactericidal Potentials

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Abstract: Over the past few decades nanotechnology is one of the most emerging areas of substantial research and metal nanoparticles have gained a great scientific interest because of their unique optoelectronic and physicochemical properties with potential applications in catalysis and drug delivery.Conventional physical and chemical methods producing metallic nanoparticles have serious drawbacks such as the involvement of toxic chemicals and the high-energy requirements for production. In this scenario, the present study has been focused on the biosynthesis of silver nanoparticles (AgNPs) using the aqueous extract of a wild edible mushroom *Termitomycesheimii*. The formation of AgNPswas observed as a colour change of the mixture from colourless to dark-brownish.Characterisation of AgNPswere done by UV-vis spectrophotometry, scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR) analysis confirmed the formation, size, shape and composition of synthesised materials. The results revealed that the AgNPsare covered with biomoieties on their surface.Aqueous extract of *T. heimii*demonstrated a great potential for the synthesis of AgNPsby rapid reduction of silver ions (Ag^{+} to Ag^{0}). Furthermore,the biofunctionalized silver nanoparticles thus produced have shown a strong bactericidal effect against *Salmonellatyphi* MTCC734 and *Shigellaflexneri* MTCC7061causingacute enteric infections in gastrointestinal tracts of human. Therefore, this 'green' method not only highlighted a simple, cost-effective and eco-friendly synthesis route of AgNPs considered for using them in many pharmaceutical applications but also explores an immense scope for developing large scale production of value added products through nanobiotechnology.

Key words: Silver nanoparticles,Eco-friendly synthesis, Pharmaceutical applications,Bactericidal effect.

P-37

Synthesis, characterization, *in vitro* antimicrobial and antimycobacterial activity of some new Schiff bases and 4-thiazolidinone derivatives as biologically active pharmacophores

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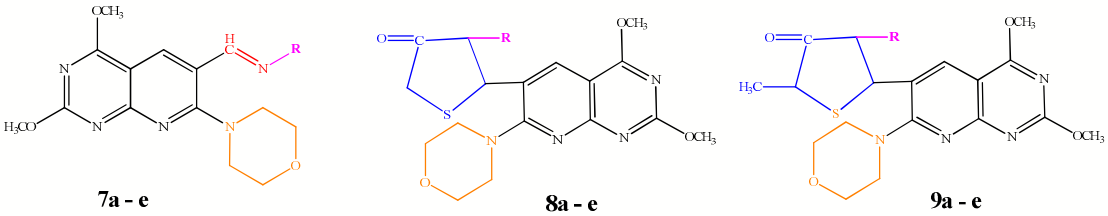
Abstract: In search for new antimicrobial and antimycobacterial agents with novel mechanism of action and enhanced biological profile, a combinatorial libraries of Schiff bases **(7a-e)**, 2,3-disubstituted-4-thiazolidinone **(8a-e)** and 2,3-disubstituted-5-methyl-4-thiazolidinone **(9a-e)** derivatives have been synthesized as new pharmacophores **Scheme 1**.



Scheme 1. Biologically active pharmacophore (**7a-e**), **(8a-e)** and **(9a-e)**

By applying standard Vilsmeier-Haack reaction condition [1], reaction of *N*-(2,6-dimethoxypyrimidin-4-yl)acetamide **(2)** with Vilsmeier-Haack reagents gives 7-chloro-2,4 - dimethoxy pyrido [2,3-d] pyrimidine-6-carbaldehyde **(3)** which on further react with morpholine **(4)** and various substituted heteroamines **(6a-e)** gives 2,4 - dimethoxy-7-morpholinopyrido [2,3-d] pyrimidine-6-carbaldehyde **(5)** and substituted Schiff bases **(7a-e)** respectively. Finally the reaction of various Schiff bases **(7a-e)** with thioglycolic acid and thiolactic acid gives 2,3-disubstituted-4-thiazolidinone **(8a-e)** and 2,3-disubstituted-5-methyl-4-thiazolidinone **(9a-e)** derivatives respectively. The structures of all the newly synthesised compounds were confirmed by their FTIR, ^{1}H NMR, ^{13}C NMR, mass spectral as well as elemental analysis data. All the newly synthesized compounds were screened for non automated *in vitro* antimicrobial [2] and antimycobacterial [3] activity against selected pathogens. Some of the newly synthesized compounds exhibited excellent antimicrobial activity and said to be the most proficient members of the series compared to standard drugs and for future scope.

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P-38

Environmentally Benign niobium chloride catalyst one-pot multicomponent synthesis of spiro[indoline-3,4'-pyrano[2,3-c]pyrazole

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Introduction

In recent days researchers are giving much importance in the synthesis of compounds with spiropyrrolidinyl-oxindole derivatives because of the presence of bioactive moieties. Even though an attempt has been made to use 4-DMAP, as a catalyst for the synthesis of spiro[indoline-3,4'-pyrano[2,3-c]pyrazole, search for novel catalyst and methodology that can lead to newer derivatives with better yield under mild conditions continues[1-2]

Experimental

Mixture of ethylacetoacetate 1 (1 mmol), 4-methoxyphenylhydrazine 2 (1 mmol), 5-bromoisatin 3 (1 mmol), ethyl cyanoacetate 4 (1 mmol) and niobium chloride 5% (by weight) in EtOH (10 mL) was stirred at room temperature for 3 h. The completion of the reaction is confirmed by using TLC.

Results and discussion

We have synthesized various spiro[indoline-3,4'-pyrano[2,3-c]pyrazole] derivatives from 5-bromo isatin and various phenyl hydrazine derivatives, ethylacetoacetate and /2-bromoacetonitrile/malononitrile/2-hydroxy-1,4-naphthaquionone. Spiro[indoline-3,4'-pyrano[2,3-c]pyrazole] was synthesized from an equivmolar mixture of 5-bromo satins, bromo acetonitrile, 4-methoxyphenylhydrazine and ethyl acetoacetate by adopting one-pot four-component reaction method .

Conclusions

We reported novel and convenient one-pot synthesis of multi-substituted spiro[indoline-3,4'-pyrano[2,3-c]pyrazole] derivatives using four-component reactions. The four component reactions proceeded smoothly and resulted in good to excellent yields. Our one-pot method offers several advantages, including short reaction time, simple experimental procedure and no toxic byproducts. The products are new heterocyclic molecules containing nitrogen, oxygen and two carboxyl groups and they may have potent biological activities.

Acknowledgements

Authors are thanks to Madurai Kamarajar University for facility of NMR instrumentation.

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P-39

Evaluation of Antileishmanial Activity of Computationally Screened Compounds Targeting DEAD Box RNA Helicase of *Leishmania donovani*

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Abstract- Visceral leishmaniasis (VL) is a life threatening infectious disease caused by *Leishmania donovani*. It leads to the severe immune suppression in the host defense system. Due to higher cytotoxicity, severe side effects and lower therapeutic indexes (TI), none of the available drugs can be considered to be ideal to treat this disease. So there is an urgent need to develop new molecules with better antileishmanial activity and high TI value. The candidate drugs should target virulent protein in parasite to inhibit its infectivity. Recently role of DEAD Box RNA helicase has been reported in survival and differentiation of virulent amastigote form of the parasite [1, 2]. So in this study, we have further evaluated DEAD Box RNA helicase as a potential drug taget by *in-silico* apporoach. We have identified 25 ligands which specifically bind to DEAD Box RNA helicase and screened them for their activity against *L. donovani*. Ten ligands performed positive interaction towards DEAD Box RNA helicase and nine showed better score than control (Miltefosine). Initially we have evaluated three commercially availabele ligands for their in-vitro antileishmanial activity. Ligand X (IC-0.5µg/ml) and Ligand Y (IC-1µg/ml) performed significantly higher antileishmanial activity against *L. donovani*. Hence, this study concludes these ligands, can be further evaluated as potential target specific drug against VL in animal model and for clinical trials.

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P-40

Post-transcriptional regulation of triose phosphate isomerase (TPI1) by miRNAs miR-22 and miR-28 with implications in hypoxia and tumourogenesis

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Triosephosphate isomerase (TPI1) is an important enzyme regulating the glycolytic flux and hence the metabolism in cells. So far, it has not been studied as to whether miRNAs, suppressing target expression by binding to the 3'UTR, regulate TPI1. The present study was conducted to investigate the regulation of TPI1, and hence the glycolytic flux by miRNAs. A bioinformatics search revealed a conserved target-site for miRNAs miR-22 and miR-28, that were downregulated in cancers, within the TPI1-3'-UTR at 499-506 and 272-277 nt respectively. An inverse correlation of miR-21 and TPI1-protein was observed across three different cell lines. Transfection of HCT-116 cells with miR-22 and miR-28 significantly suppressed a luciferase-reporter containing the TPI1-3'-UTR which was abolished when a construct mutated at the miR-22/nt 499-506 and miR-28/nt 272-277 target site was used instead. Moreover, overexpression of miR-22 and miR-28 in HCT116 significantly reduced the endogenous TPI1-protein amounts. Anti-miR-22 and Anti-miR-28, when transfected, were found to abolish this inhibition of miRNAs on the endogenous TPI1 protein levels. Resected normal/tumor tissues of 30 colorectal cancer patients demonstrated an inverse correlation between miR-22/miR-28 and TPI1-protein. miR-22/miR-28 transfected HCT116 cells were also shown have reduction in the secretion L-lactate levels reflective of the inhibition of the glycolytic flux by the said miRNAs. The inverse correlation between the said miRNAs and the TPI1 protein was also observed upon hypoxia with the former downregulated and the latter upregulated. This is the first study to show that TPI1 is negatively regulated by miR-22/miR-28 which act as tumour suppressor miRNAs.

Keywords: TPI1; miR-22, miR-28; post-transcriptional regulation; L-lactate, hypoxia.

P-41

GC-MS based phytochemical screening of normal butanol extracts from the leaves of *Grewia tenax*, Kachchh region, Gujarat

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Abstract: *Grewia tenax* (GT) is the mutual name of Guddaim or Gangeti, a treasured plant species in Kachchh region.Leaves of *G. tenax* are a significant part of traditional remedy for the use of treatment against tonsillitis infections, trachoma and are used as a compress against inflammation. *Grewia's* extracts are also useful in remedial hepatitis and other such type of diseases. The plant contain high therapeutic values and is used for treatment of several diseases such as dysentery,fever, rheumatism, diarrhoea, anaemia, osteoporosis, body weakness nausea, bone fractures, and for bone and muscular strengthening.The present study has been carried out on the analysis of the major bioactive components of therapeuticallysignificant plant *Grewia tenax* (GT) leaves by use of GC-MS (Gas Chromatography–Mass Spectrometry),whereas the mass spectra of the compounds found in the extract was corresponding with the NIST(National Institute of Standards and Technology) library. The soxhlet extraction of sample was done by use of continuous hot percolation method using n-butanol as a solvent. After extraction it was concentrated by use of distillation method. Crude n-butanol extracts were introduced in GC-MS instrument for isolation and identification of valuable phytochemicals. GC-MS analysis showed the presence of twenty five compounds. The result exhibited that there are very significant phytochemicals found in n-butanol leaves extract of *G. tenax* like alkaloids, sterols, lipids, glycerol phospholipids, fatty esters, fatty acid, glycoside, carotene, steroidal alkaloid, triterpene glycosides, glycerol phosphate sand sesquiterpenes.

Key words: *Grewia tenax*, GC-MS, Phytochemicals, n- butanol extract, Soxhlet extraction

P-42

Phytochemical Analysis of Chlorobenzene leaves Extract of *Abutilon pannosum*for Its Bioactive Components through Gas Chromatographic Mass Spectrometry (GCMS)

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Abstract: *A. pannosum* usually recognised as khapat is a significant therapeutic plant used in a traditional system. Its extract is also used in treating against bronchitis, gonorrhoea, diarrhoea in relieving thirst, and inflammation of the bladder and in reducing fever, cleaning wound and ulcer, treating a vaginal infection, diabetics, haemorrhoids and can also be used as an anaemia. The present study has been carried out on the analysis of the major bioactive components of therapeutically significant plant *Abutilon pannosum* (A.P.) leaves by use of GC-MS (Gas Chromatography–Mass Spectrometry), whereas the mass spectra of the compounds found in the extract was corresponding with the NIST (National Institute of Standards and Technology) library. The soxhlet extraction of the sample was done by use of continuous hot percolation method using chlorobenzene as a solvent. After extraction, it was concentrated by use of distillation method. Crude chlorobenzene extracts were introduced in GC/MS instrument for isolation and identification of valuable phytochemicals. The GC-MS analysis showed the presence of 15 compounds. The result exhibited that there are very significant phytochemicals found in Chlorobenzene leaves extract of *A. pannosum* like alkaloids, sterol lipids, glycerophospholipids, fatty ester, fatty acid, glycoside, carotene, steroidal alkaloid, triterpene glycosides, glycerophosphates, sesquiterpenes and phosphatidylglycerol.

Key words: Abutilon pannosum, GC/MS, Phytochemicals, Chlorobenzene extract, Soxhlet extraction

P-43

Synthesis, Fluorescence and Antioxidant Activity of Ethenyl Indoles

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Living organisms uptake oxygen for cell metabolism, which produces reactive oxygen species (ROS). Various human diseases such as cancer, heart disease, atherosclerosis, etc might occur due to ROS induce cell damage. Antioxidant protects these cell by scavenging the reactive oxygen species and thus play important role. Though many nitrogenous and hydroxyl based conjugated molecules are well known for scavenging the ROS, the understanding of mechanism of anti-oxidation is not very clear. In this context, we have synthesized various donor-acceptor substituted ethenyl indoles {e.g. 3-(4-nitrophenylethenyl-*E*)-N-H-indole (**1**), 3-(4-chlorophenylethenyl-*E*)-N-H indole (**2**), 3-(4-phenylethenyl-*E*)-N-H indole (**3**), etc}, and studied their excited state properties, antioxidant activity and discussed a possible mechanism for anti-oxidation. It is shown that the excited state of ethenyl indole (**1**) bearing a strong electron acceptor substituent is highly dipolar and fluorescent in nature and do not shows antioxidant activity, whereas, other ethenyl indoles exhibit comparable antioxidant activities as compared to vitamin C and vitamin E. We have discussed the possible mechanism for antioxidant activity. In addition to this, these ethenyls interacts with Bovine serum albumin with binding constant in the range of 1-10 (10^5 M^{-1}). These information provide useful information in understanding the excited state properties and designing of newer conjugated molecules with medicinal properties.

P-44

Mixed Micelle Formation in an Aqueous Mixture of Surfactants: A Thermodynamic & Theoretical Study

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ABSTRACT: Mixed surfactants have been extensively studied in recent times in the various combinations of conventional cationic, anionic surfactants, gemini surfactants, zwitterionic and non-ionic surfactants. In technology mixed surfactants are used in phermacuticals, detergency, foods, cosmetics, solubilisation of drugs and enhanced oil recovery. We have studied the interaction between a **S**urface **A**ctive **I**onic **L**iquid (**SAIL**) with a convensional surfactant (DTAB), at 303.15 K with different mole fractions. Using the well established models such as Clint, Rubingh and Motomura, ideal *cmc*s (critical micelle concentration) in mixtures, various interaction parameters, miceller mole fractions and activity coefficients have been calculated theoretically. It has been seen that the experimental *cmc*s of the mixed surfactants differ significantly from the theoretical values. This observation reveals that the formation of mixed micelle does not follow the ideal behaviour of mixing. The values of negative interaction parameters for different mole fractions of the system suggest that the interaction of SAIL with surfactant is synergistic and it increases with the increase of surfactant contents. The free energy and enthalpy values are found to be negative for all compositions with increase in mole fractions of investigated surfactant.

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P-45

CTAB - SDS interacted catanionic system in aqueous medium at below, near, and above their critical micelle concentrations (CMCs): A Multifarious physicochemical investigation

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Abstract: Interaction between cetyltrimethylammonium bromide (CTAB) and sodium dodecylsulfate (SDS) has been studied to understand the types of self-assemblies formed in aqueous medium. Three different concentrations below, near, and above CMC (critical micelle concentration) of both surfactants have been studied up to their equi-molar proportions, and above. Mixed micelles, normal and distorted bilayers, and curved bilayer assemblies (or vesicles) were found to form. Formed CH_3 $(CH_2)_{15}$ $CTA^{+-}SD$ $(CH_2)_{11}$ CH_3 (catanionic surfactant species) was produced in solution without precipitation. At a specific low << 1:1 molar proportion, faintly bluish translucent solution was formed. This was the critical vesicle concentration (CVC) supported from turbidimetry, conductometry, and calorimetry measurements. The dimensions of the formed vesicles (by the addition of SDS to CTAB and vice versa) were found from dynamic light scattering (DLS), fluorescence anisotropy measurements. The formed vesicles at 1:1 composition at different surfactant concentrations were very stable; they were non-sticky, milky white texture, and low viscous. Addition of methanol, ethanol, iso-propanol, tetrahydrofuran, and dimethylsulfoxide in fairly high proportions made the turbid solutions clear. FESEM and CFM evidenced formation of ion-pair products as well as both uni-, and multi-lamellar vesicles of moderate and large prolate sizes. The antibacterial properties of the vesicles were also tested against E. Coli and B. Subtilis with fair inhibition activities. The study has a multifarious projection objective.

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Study on Phytochemical properties of *Hippophae salicifolia* leaves of Uttarakhand region

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Abstract: *Hippophae salicifolia* (Seabuckthorn) is well known for its extraordinary medicinal potential due to the presence of various antioxidant components such as Vitamin E, tocopherols, flavanoids etc. Whole plant has numerous nutritional benefits and the plant is also stress tolerant as well as excellent soil stabilizer and used as fodder additives. The present study was conducted to examine antioxidant potential of methanolic extract of seabuckthorn *(Hippophae salicifolia)* leaves harvested in the month of July 2016 at Auli, Chamoli district of Uttarakhand. The leaves were shed dried for 10 days and grinded in mixer. The phytochemical analyses of the secondary metabolites including phenolics, flavanoids and free radical scavenging activity were measured in methanolic extract of the plant. The extract was prepared by Soxhlet apparatus and solvent evaporation was done using Rotary evaporator. The results revealed that *Hippophae salicifolia* leaves contains FRSA 21% , total phenolics 77 µg/ mg GAE and total flavanoids 69 µg/ mg of QE. Further, chemical characterization of the extract was carried out using GC – MS which showed the major component in seabuckthorn leaves were cis-9-hexadecenal (13.53%), linoleic acid (12.34%), inositol (12.12%), palmitic acid (5.33%), β–D-glycopranoside (5.17%), hexadecanoic acid (4.3%), Vitamin E (2.91%) and hydroquinone (2.3%). The other important constituents like squalene, docasanol, oleic acid, phytol etc were also found in minor quantities. Thus, the present investigation indicates phytochemical properties of *Hippophae salicifolia* leaves having high medicinal significance.

Keywords: *Hippophae salicifolia* leaves, methanolic extracts, phytochemicals, antioxidant components, GC-MS

P-47

Development and Validation of a Rapid Chemometrics Assisted RP-HPLC Method for the Simultaneous Estimation of Ciprofloxacin and Ornidazole in Bulk and Pharmaceutical Dosage Form

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ABSTRACT: Simple, rapid, precise, and accurate RP-HPLC method was developed and optimized with the help of chemometric tool for the simultaneous estimation of Ciprofloxacin and Ornidazole in bulk and pharmaceutical dosage form. Optimization was done by central composite design in response surface methodology. Based on the trial and error, percentage of organic phase (Acetonitrile) in mobile phase, flow rate, and molarity of the buffer were selected as factors. Resolution and retention time were used for the estimation of system response during the optimization procedure. The optimized condition was used and the separation was carried out on phenomenex C_{18} column (150 × 4.6 mm; i.d, 5 µ particle size) using the mobile phase containing 62% of Acetonitrile and 38% of acetate buffer (0.1 mM) at a flow rate of 1 mL/min. Retention time was found to be 1.3 minutes for Ciprofloxacin and 3.8 minutes for Ornidazole. The calibration curves were found to be linear from 20 to 120 µg/mL and 10 to 60 µg/mL for Ciprofloxacin and Ornidazole with their correlation coefficient values 0.9997 and 0.9998. LOD and LOQ were found to be 32.2 ng/mL and 96.1 ng/mL for Ciprofloxacin and 41.9 ng/mL and 152.6 ng/mL for Ornidazole.

Keywords: Central Composite design, Ciprofloxacin, HPLC, Ornidazole, Validation

P-48

Design, synthesis and evaluation of anti-inflammatory activity for condensed thienopyrimdine derivatives

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Abstract: A series of virtual chemical library from condensed thieopyrimidine derivatives were subjected to molecular docking for development of novel anti-inflammatory agent. The molecules possessing better binding affinity against COX were selected, synthesized and evaluated for their antiinflammatory activity against carrageenan induced oedema in wistar rats. The general synthetic pathway to the thieno[2,3-*d*]pyrimidin-4(3*H*)-ones were synthesized by condensations of 2-aminothiophene carboxylate and formamide. The 4-chlorothieno [2,3-*d*]pyrimidines was prepared by the chlorination of thieno[2,3-*d*]pyrimidin-4(3*H*)-ones with Phosphorous oxychloride in good yield. Microwave fusion of 4-chlorothieno [2,3-*d*]pyrimidines with *o*-phenylenediamine afforded the target compounds. The structure of compounds was confirmed by IR, 1H-NMR and mass spectral data. The test compounds had higher percent of inhibition of oedema at a dose of 20 and 30 mg kg–1 oral. All the tested compounds showed promising antiinflammatory activity. Two compounds among the series were most active than the standard diclofenac.

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P-49

Synthesis and anticancer studies of novel thieno pyrimidine containing pyrrolidine-2-carboxylic acid amides

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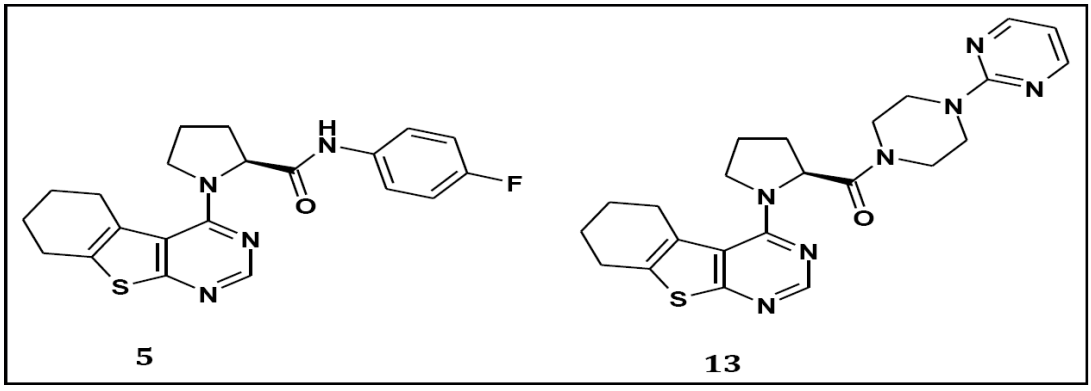
Abstract : Tyrosine kinases inhibitors, that has been introduced in recent years is directed against cancer-specific molecules and signalling pathways with some side effects. Tyrosine kinases are orally active, small molecules that have a favourable safety profile and can be easily combined with other forms of chemotherapy or radiation therapy. Several tyrosine kinase inhibitors such as gefitinib [1] erlotinib [2] and lapatinib [3] have gained market approval worldwide. Therefore, we studied these classes of molecules to obtain new candidates of remarkable activities and minimal side effects.



We have prepared a series of new thieno [2, 3-d] pyrimidines by introducing a five member cycloalkyl ring containing secondary nitrogen (L- proline) at C-4 position of the *5,6,7,8-Tetrahydro-benzo[4,5]thieno[2,3-d]pyrimidine* & synthesized pharmacophoric amide moieties of interest that proved to contribute for antitumor activities. Compounds **5** and **13** showed descent antitumor activities when compared to Doxorubicin (*GI50* < 0.1) for human Breast cell line MCF-7.

Key Words : Tyrosine kinases inhibitors, thieno [2, 3-d] pyrimidines , anticancer activity

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P-50

Pharmacological evaluation of novel PKR inhibitor Indirubin-3-hydrazone in H9C2 cardiomyocytes.

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Abstract: Double stranded protein kinase R cellular response is associated with various stress signals such as nutrients, endoplasmic stress, cytokines and mechanical stress. Increased PKR activity has been observed under diabetic and cardiovascular disease conditions. Most of the currently available PKR inhibitors are non-specific and have other effects as well. Thus, the aim of the present study was to examine the effect of novel PKR inhibitor indirubin-3-hydrazone (IHZ) in cultured rat H9C2 cardiomyocytes and to investigate whether inhibition of PKR could prevent any deleterious effects of high glucose treated cells. PKR expression was determined by Q-PCR, immunofluorescence and immunoblotting. The expression of different gene markers for apoptosis was measured by RT-PCR. Apoptosis and oxidative stress were determined by flow cytometry. High glucose treated H9C2 cardiomyocytes developed a significant increase in PKR expression. A significant increase in apoptosis and generation of reactive oxygen species was also observed in high glucose treated H9C2 cells. Reduced vacuole formation and prominent nuclei was also observed in high glucose treated cells. All these effects of high glucose were attenuated by novel PKR inhibitor, indirubin-3-hydrazone. Our results indicate IHZ as an effective inhibitor of PKR *in vitro* in cultured cardiomyocytes and thus it may prove very useful in blocking the multiple deleterious effects of PKR.

Key words: Indirubin-3- hydrazone, High glucose, Cardiomyocytes.

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P-51

Synthesis and biological evaluation of some newly synthesized barbiturates and their derivatives using task specific ionic liquid [Bmim]OH

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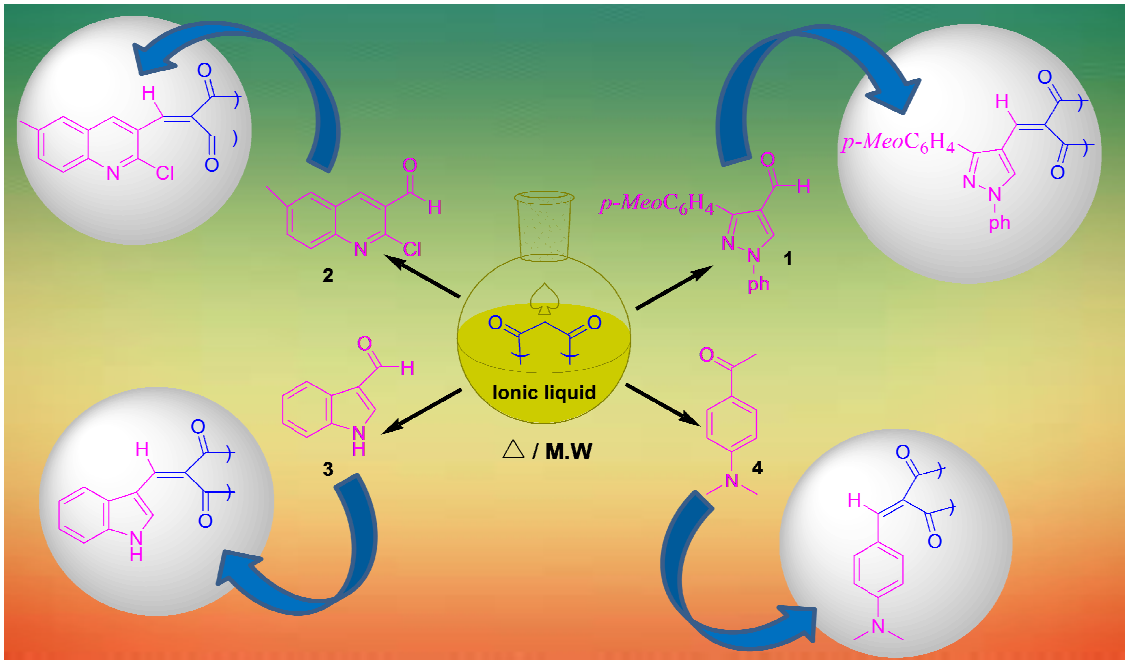
Graphical Abstract:



Eco-friendly synthesis of some selected Barbiturates, Thobarbiturates and Dimedone derivatives has been developed by using task specific ionic liquid Bmim[OH], which not only act as catalyst but also the best solvent media for the knovengeal condensation reaction between heteroaryl (pyrazole, 2-chloro-quinoline and Indole) aldehydes with barbituric/ thiobarbituric acid and dimedone. High yield and less reaction time are the advantages of this methodology. All the synthesized compounds were tested for their antimicrobial activities. Most of the compounds showed very good antibacterial and antifungal activity.

Keywords: 1-Butyl-3-methyl-midazolium hydroxide, Barbituric acid, Quinoline, Dimedone, Antimicrobial activity.

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P-52

SELECTIVE DETECTION OF AZINPHOS-METHYL PESTICIDE BY A CADMIUM BASED FLUORESCENT METAL ORGANIC FRAMEWORK

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A metal organic framework (MOF) **[Cd_3 (PDA)$(tz)_3Cl(H_2O)_4$].$3H_2O$** (PDA=1,4-Phenylenediacetate, tz=1,2,4 triazole), **Cd@1**, has been synthesized at room temperature. The structure of **Cd@1** was characterized systematically by X-diffraction method, Thermogravimetric analysis (TGA) and Infrared spectroscopy(IR). Photoluminescence study of **Cd@1** in aqueous medium showed emission at 290 nm upon excitation at 225 nm. This emissive property was used for the detection of pesticide residues through luminescence quenching. The **Cd@1** is highly selective and sensitive towards pesticide Azinphos-Methyl even to the lowest limit of 8 ppb. It's sensitivity and selectivity remains unaltered in presence of surfactants (SDS and CTAB) as well as in presence of fruit and vegetable extracts (Apple and Tomato). The sensitivity remains unaffected in presence of other pesticides like Chlorpyrifos, Dichlorvos, Endosulfan, Diazinon , Malathion and Parathion.

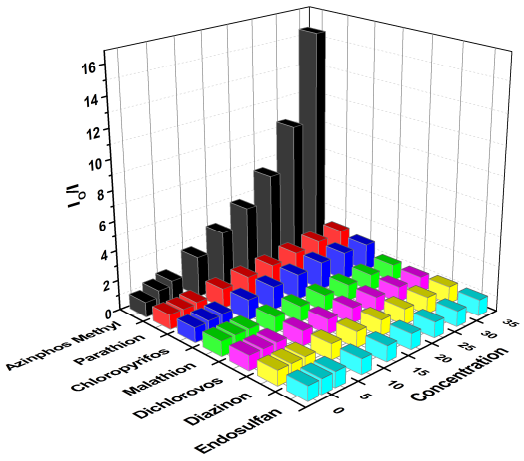

Fig-1: Emission spectra of Cd@1 dispersed in H_2O upon incremental addition of 1 mM Azinphos-. λ_{ex} = 225 nm; The final concentration of Azinphos-methyl is indicated in the legend

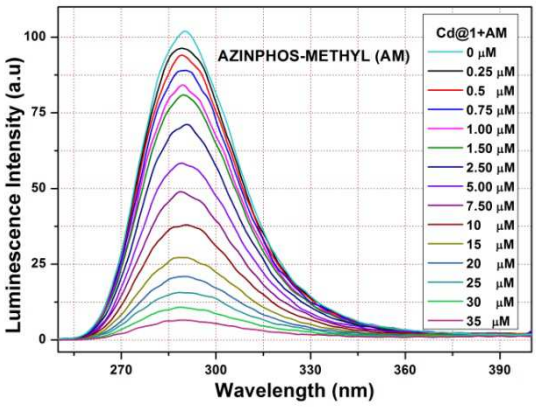

Fig -2: Stern-Volmer plots of Cd@1 in presence of different Pesticides

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P-53

TOWARD THE SYNTHESIS AND PHARMACOLOGICAL SCREENING OF A NATURAL CYCLOPOLYPEPTIDE FROM PLANT ROOTS

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ABSTRACT: The solution-phase synthesis of a proline and glycine-rich plant-derived cyclic heptapeptide, gypsophin E (**8**) is reported *via* coupling of tetrapeptide unit Glycyl-L-leucyl-L-valyl-L-proline-OMe with tripeptide unit Boc-L-isoleucyl-glycyl-L-proline-OH followed by cyclization of the linear fragment having seven amino acid units. The structure of the newly synthesized cyclic heptapeptide as well as that of the intermediate tri/tetra/heptapeptides was confirmed by FT-IR, ^{1}H NMR, ^{13}C NMR spectroscopy and elemental analysis. In addition, mass spectra were recorded for the cyclic heptapeptide and further, subjected to the antimicrobial and the anthelmintic activity studies. It was evident from the pharmacological activity results that the newly synthesized cyclopolypeptide displayed potent antifungal and anthelmintic activities against the pathogenic fungi *Candida albicans*, the dermatophytes *Trichophyton mentagrophytes*, *Microsporum audouinii* at 6 µg/mL level and the earthworm species *Megascoplex konkanensis*, *Pontoscotex corethruses* and *Eudrilus eugeniea* at the concentration of 2 mg/mL.

KEYWORDS: Gypsophin E, Cyclic heptapeptide, Peptide synthesis, Macrocyclization, Antimicrobial activity, Anthelmintic activity.

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P-54

Novel methods for the fusion of pyridine ring in steroidal moiety: Application of Vilsmeier reaction, Michael addition and [4+2] cycloaddition reaction

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The modification of steroid with a heterocyclic ring is a subject of much interest as numbers of steroidal compounds having a heterocyclic core are found to have biological and pharmacological applications[1-2]. Hence efforts are being made to fuse pyrazole, isoxazole, pyridine, pyran, pyrrole, pyrimidine, thiazole, isothiazole rings with steroidal moiety using various synthetic strategies [3]. A few methodologies including Vilsmeier reaction [4], Michael addition [5] and [4+2] cycloaddition reaction [6] are reported herein to synthesize some pyridine fused steroids.

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6. Manuscript under submission

P-55

Study of L-Glutaminase Production by *Acinetobactercalcoaceticus* PJB1 and Antioxidant Activity of Fermented Hydrolysate

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Abstract: Antioxidant compounds play an important role against various diseases like chronic inflammation, atherosclerosis, cancer and cardiovascular disorders and ageing processes. In this study, a glutaminase producing isolate *Acinetobactercalcoaceticus* PJB1 was grown in sugarcane bagasse solid substrate. The optimum glutaminase production (113.53 U/gds) was observed at pH, 10.0; temperature, 35°C; inoculums concentration, 1.0% (v/v); incubation period 72h and sugarcane bagasse concentration 6% (w/v). The fermented hydrolysate was collected by membrane filtration (100 KDa) andamino acids were analyzed through HPLC that signifies the presence of adequate amount of glutamic acid. Free radical scavenging activity of fermented hydrolysate was conceded using a DPPH and FRAP assay comprising IC_{50} value of 41.14µg/ml and 47.97µg/ml respectively, for determination of the antioxidant capacity. These findings may facilitate novel applications of fermented hydrolysate in food and pharmaceutical industries.

Keywords: Glutaminase, antioxidant, fermented hydrolysate, DPPH, FRAP

P-56

Assessment of Biochemical andMolecular Variability of Plant Growth Promoting Antagonistic Fluorescent Pseudomonadsof West Bengal, India

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Abstract: Twenty-five native Pseudomonads were isolated from rhizosphere of tomato plants from gangetic old alluvial, terai, gangetic new alluvial and coastalregionof West Bengal. The isolates were characterized by 16s r-RNA gene sequencing and phylogenetic analyses. Among the fluorescent Pseudomonads, *Pseudomonas aeruginosa* was found to be dominant (28%), followed by *P. monteilii* (24%). Least abundant species were *P. moselii* and *P. cepacia* (8%). Different molecular fingerprinting tools such as ARDRA, ERIC-PCR, BOX-PCR were applied to define their genotypic diversities. Restriction analysis (ARDRA) of *Pseudomonas* genus specific 618 bp DNA fragment was performed with four tetra cutters, *Hae* III, *Hinf* I, *Msp* I and *Taq* I. Among them, the combined effect of *Msp* I and *Hae* III, tested, could efficiently differentiated the strains to their species level to much extent. This is probably the first report of restriction finger printing of the 618bp Pseudomonads genus specific DNA fragment. All the strains showed wide variations in fingerprinting pattern in ERIC and BOX- PCR assays. In BOX- PCR assay a unique banding profile for *P. aeruginosa* group was observed. An attempt was taken to develop a PCR- DGGE system that specifically described the diversity of Pseudomonads directly from soil. The results revealeddifferences in the composition of Pseudomonas community structures between the regions.Higher diversities, (Shannon-Weaver indices) were consistently observed in the soil samples from old alluvial regionfollowed by terai region. Thus knowledge generated on biodiversity of antagonistic fluorescent Pseudomonads bacteria will provide a new strategy for biological control from ecological viewpoints.

Keywords: Rhizosphere, Pseudomonads,DGGE

P-57

Phyloproteomics of Tannase and Amino Acids Conservancy in Catalytic Site: An *In Silico* Docking Analysis

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Abstract: Recently, tannase have gained an enormous importance in food, pharmaceutical and beverage industries as it efficiently removes the toxic effects of plant phenolic compounds from consumable products by breaking ester and depside bonds. Gallic acid, the hydrolyzed product of tannase action, has potent medical as well asindustrial applications. In this study 1277 tannase protein sequences were retrieved from NCBI and on the basis of sequence divergency 625 sequences were selected belonging to 78 bacterial and 20 fungal genera. Based on the phylogenetic analysis and species abundance 380 sequences were taken for tertiary structure prediction and among them 46 quality structures were used for structure based phylogenetic tree construction and molecular docking study. In structure based phylogeny enteric and nonenteric tannase were distinctly found in two different groups. Structural comparison revealed differences at the lid domains, whereas the presence of 9 β-sheet conserved secondary structure was observed within all types of tannase. The conserved catalytic triad S-D-H, forming direct H-bonds with the substrates, was found in all the docked structures. The functional similarity with sequential diversity among different tannases indicated their orthologous relationships. Tannin and ferulic acid are both phenolic derivatives of plants and possess ester bonds.More than 70% tannase sequences showed both tannase and feruloyl esterase activity despite of their lid domains structural diversity. Moreover, the study revealed that tannase allows substrate variability but maintains catalytic specificity.

Keywords: Tannase, Molecular docking, Catalytic triad, Structural diversity

P-58

Synthesis, characterization and application of versatile ZnO@SnO_2 mixed metal oxide nanoparticles for the synthesis of Hantzsch 1,4-dihydropyridines

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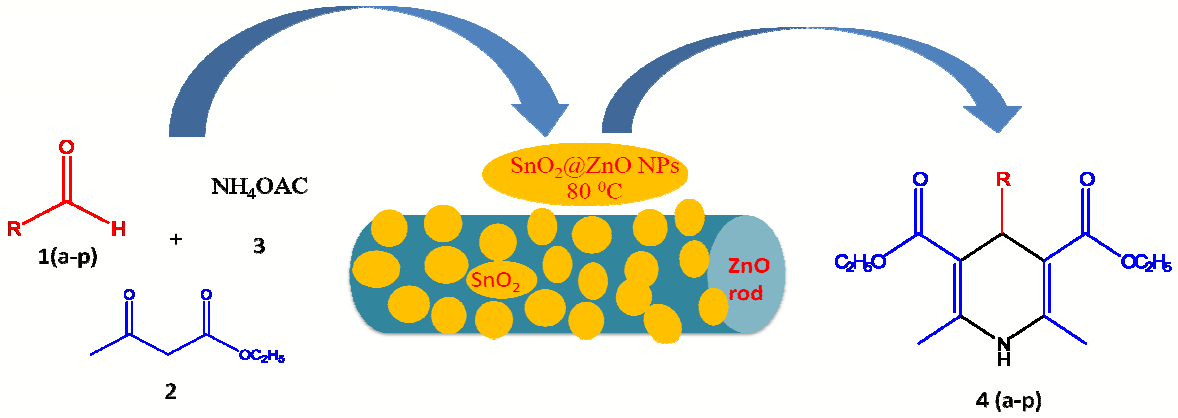
Abstract: An efficient synthesis of Hantzsch 1,4-dihydropyridines *via* a one-pot three-component reaction of ethyl acetoacetate, substituted aldehydes and ammonium acetate in the presence of ZnO@SnO_2 mixed metal oxide under solvent-free conditions was reported. This method shows attractive characteristics such as; cleaner reaction profiles, short reaction times, little catalyst loading and high yields. Isolated catalysts were reused for new reactions without considerable loss of their catalytic activity. The catalyst was characterized by FT-IR, XRD, EDX and SEM analysis.

Graphical Abstract:



Key words: 1,4-dihydropyridines, One-pot multi-component reaction, ZnO@SnO_2 nanoparticles, Solvent-free,

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Keratinase of *Bacillus weihenstephanensis* PKD5: Purification and Potential Applications in dehairing of skin and hide

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Abstract

Chicken feathers as poultry by-product have been creating a serious environmental pollution due to its recalcitrant nature. A keratinase producing bacteria as *Bacillus weihenstephanensis* PKD5 (JN897383) was newly isolated from feather dumping site of Midnapore, West Bengal, India. SEM study showed the average length and diameter of the strain as 3.5 µm and 0.8 µm respectively. Optimization of cultural conditions in submerged fermentation scaled up the production of keratinase upto 15.3 U/ml. The keratinase production was further enhanced to 164.9 U/g through RSM optimization, which was 3.17 fold higher.

The extracellular keratinase was partially purified by ammonium sulphate precipitation (80% saturation) with a purification fold of 1.3888 and 60.42% yield. The enzyme was further purified throughSephadex G-100 Column with purification fold of 5.32, yield 42.95%, specific activity 462.81 U/mg and total protein 142 mg. Purification homogeneity was achieved by HPLC with single peak. The molecular mass was found as 56.4 kDa by SDS-PAGE. The exact MW was found as 56427.53 Da through MALDI-TOF analysis. The enzyme was serine type protease as it was inhibited by PSMF.

The crude keratinase of *B. weihenstephanensis* PKD5 was explored as dehairing agent of skins and hide. Comparative studies among different dehairing agents (chemical and enzyme) were carried out which revealed that keratinase alone was able to perform complete dehairing within 10 h at room temperature (pH 8.0) and at an concentration of 15.3U/ml. The bacterium *Bacillusweihenstephanensis* PKD5 has a great biotechnological potential as a novel and eco-friendly keratinase producing organism.

Keywords: *Bacillus*, Keratinase, Purification, Deharing.

P-60

Design and synthesis of novel phenothiazine festooned dihydropyrimidines as anti-tubercular agents

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Abstract: Tuberculosis (TB), caused by the pathogenic Mycobacterium tuberculosis (Mtb), is one of the deadly diseases and the number of people infected by Mtb is currently estimated to be 2−3 billion worldwide. It is known that TB is registered in almost all the developing and under developed countries, however, two asian countries such as China and India together alone accounted for 40% of total TB cases worldwide. Although there are drugs available to utilize for this deadlier disease, development of new drugs for the same or development of new intermediates for further construction towards the targets for this disease is highly essential due to various reasons. Having the importance of developing new classes of molecules as anti-tubercular agents in mind, we designed and synthesized a series of new heterocyclic molecules which possess heterocyclic phenothiazine and dihydropyrimidine structural motifs in addition to amide units. The aforementioned series, phenothiazine derivatives bearing dihydropyrimidine nucleus, have been synthesized via Biginelli multi-component reaction. All the synthesized new chemical entities of 4-(10-alkyl-10H-phenothiazin-3-yl)-6-methyl-2-oxo-N-2,3,4-substitutedaryl-1,2,3,4-tetrahydropyrimidine-5-carboxamide compounds have been characterized by FT- IR, ^{1}H NMR, and ^{13}C NMR spectroscopy. Further, preliminary anti-tubercular activity against Mycobacterium tuberculosis (Mtb) has been evaluated.

Keywords: MCR; DHPM; M.tuberculosis; TB agents

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P-61

Pd-Catalyzed Cross-Coupling Reaction of Bromo-Chalcones with Ethyl Acetohydroxamate

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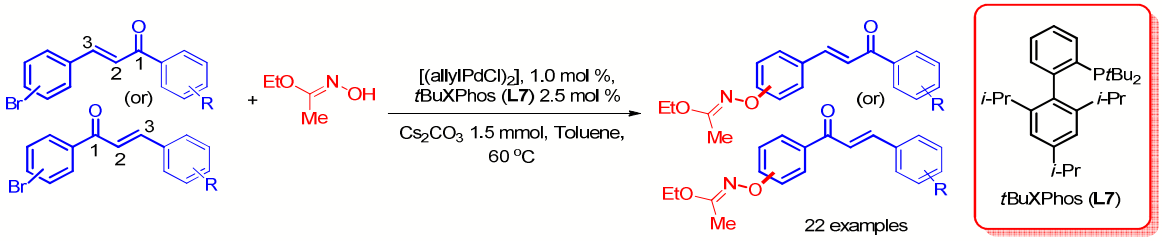
Abstract: O-arylatedethylacetohydroxamates have recently been used as useful synthetic precursors for the synthesis of benzofurans. An efficient Pd-catalyzed C-O cross-coupling of 4-bromo-chalcons and ethylacetohydroxamate has been developed and a variety of 4-bromo-chalcones have been coupled with ethylacetohydroxamate, under optimized reaction condition, in good to excellent yields. [(π-ally PdCl)$_2$] and *t*BuXPhos ligand catalyst system has found an efficient catalyst system for this coupling. However this catalyst system is failed to couple 3-bromo-chalconswithethylacetohydroxamate which substantiates that this catalyst system allows the reductive elimination step through electronic pathway.



P-62

One-pot acid mediated Indole-ring opening/ N-formylation or N-acylation cascades to pyrazolo[3,4-b]pyridin-5-yl)phenyl)formamide and pyrazolo[3,4-b]pyridin-5-yl)phenyl)acetamide derivatives

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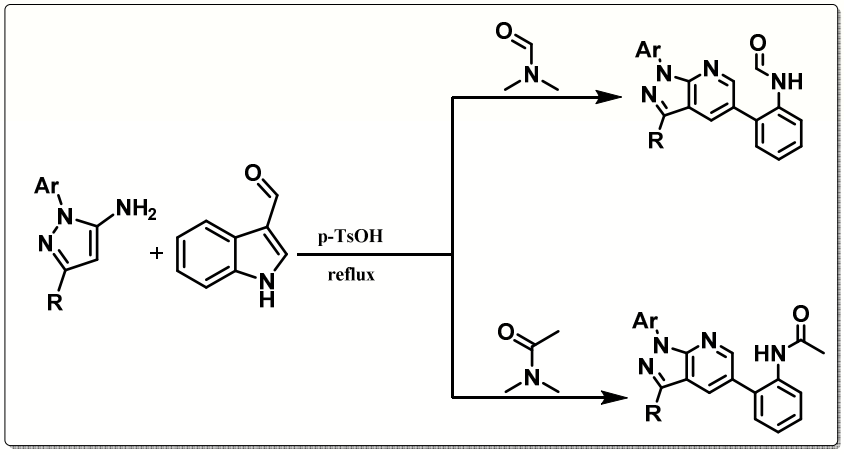

Abstract: A highly efficient one pot method was developed for the synthesis of **pyrazolo[3,4-b]pyridin-5-yl)phenyl)formamide** and **pyrazolo[3,4-b]pyridin-5-yl)phenyl)acetamide** derivatives.[1] An acid mediated cascade reaction occurred through two consecutive step, first the indole ring opening, which was further followed by insitu N-formyltion or N-Acylation in the presence of DMF or DMA, which acted as both the solvent and as formylating and acylating reagent [2] in presence of an acid.

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P-63

Ag(I)-Catalyzed Cycloisomerization Reactions: Synthesis of Substituted Phenanthrenes and Naphthothiophenes

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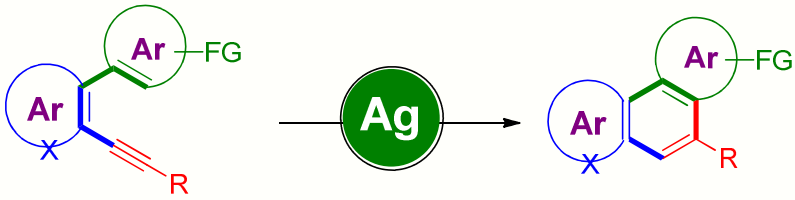

Ag-catalyzed synthesis of substituted phenanthrenes and naphthothiophenes from ortho-alkylated biaryl derivatives via 6-*endo-dig* intramolecular alkyne-arene coupling has been described. The mechanistic study reveals that 6-*endo-dig* cyclization proceeds through initial π-coordination of the alkyne unit followed by a Friedel–Crafts-type electrophilic aromatic cyclization at the adjacent arene ring. X-ray crystallographic studies further supported the formation of carbocycles.

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P-64

A Copper Catalysed Cascade synthesis of new Quinazolinone derivatives: *in vivo* Antidiabetic Activity, Molecular DFT and Docking Study.

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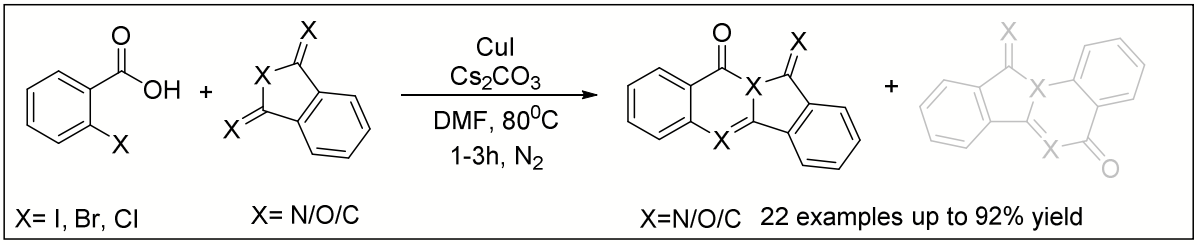
Quinazolinones are important class of heterocyclic compounds which are commonly found in many natural products and pharmaceuticals.[1]In addition to a variety of biological activities that quinazolinone alkaloids possess, cytotoxicity is a frequently found property in several members of this alkaloid family, as exemplified by luotonin F (2),[2]luotonin A (3),[2b,3] and fumiquinazoline A (4).[4] Moreover, the quinazolinone moiety has been extensively utilized as a drug like scaffold in medicinal chemistry, and as such, the quinazolinone skeleton is considered to be a privileged structure.[5] Considering the importance of the quinazolinone motif , herein we introduce a novel , simple and efficient synthesis of 12-iminoisoindolo[1,2-b]quinazolin-10(12*H*)-ones by a copper catalysed cascade reaction of 2-halobenzoic acids and isoindoline derivatives. The reaction involves bond formation of a new imino-carbon bond and a C-N bond in a one-pot mildly operable conditions under nitrogen atmosphere to afford the products in good to excellent yields. Various functional groups along with sensitive groups were tolerated under the employed reaction conditions. The as-made compounds showed promising *in vitro* antidiabetic activity in swiss albino mice. Molecular DFT and docking studies helped us in understanding the stability and structure activity relationship respectively.

General Scheme:



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P-65

Alpha carbonyl assisted unprecedented applications of 2-oxoaldehydes and malonate half esters via common Aldol Intermediate.

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Inspired by nature that uses carboxylic acids/carbonates as antecedents to carbon nucleophiles in a variety of reactions, synthetic chemists have imitated this process to perform a different decarboxylative carbon-carbon bond formation using a variety of substrates.[1] However, the condensation reaction is not feasible in the absence of a promoter. As an exception, it is a well established fact that in 2-oxoaldehydes (OAs), the higher reactivity of aldehydic group in comparison to normal aldehydes is attributed to the existence of an electron-withdrawing ketone group and has been well explored to produce different important structures.[2] This highlights a distinct feature of OAs that led to the generation of selective products through base controlled reactivity of the Aldol intermediate formed between 2-oxoaldehydes and malonate half esters (Figure 1). Previously, different groups have established the synthesis of α,β-unsaturated esters using different carbon-carbon bond forming strategies.[3] A significant drawback of these methods is their modest atom economy and use of expensive substrates. In addition the aza- Michael addition of azoles to *α,β*-unsaturated carbonyl compounds for the generation of *β*-azolated structures is a well explored reaction (Figure 1).[4] However, selective synthesis of *α*-azolated product is still a challenge.

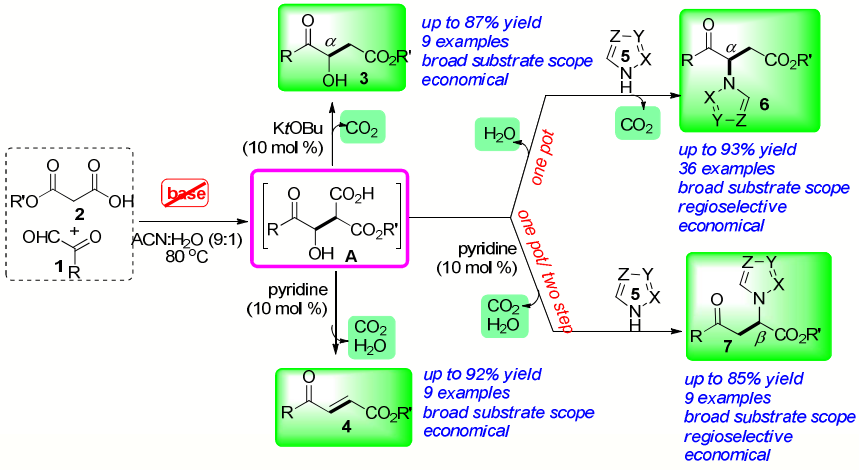

Figure 1: Summary of our work

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P-66

Nurturing a novel methodology for the synthesis of oxadiazaboroles

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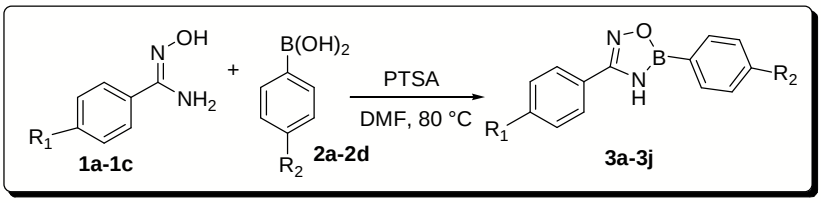
Amidoximes are versatile precursors of many heterocyclic compounds of pharmaceutical importance. On the other hand, aryl boronic acids and their esters are highly popular as synthetic intermediates in organic synthesis with their ease of conversion to other functional groups (such as phenols and aryl halides) with a well-known reaction. Literature survey of oxadiazaboroles from the above precursors i.e. amidoxime and aryl boronic acid reveals that only a limited number of reports were given in 1960s and 1970s at without any spectral data provided for those hetero cycles.

In continuation of our studies in developing inexpensive and environmentally benign methodologies for the synthesis of bioactive molecules, herein, we report a novel and direct synthesis of 5-disubstituted 1,2,4,5- oxadiazaboroles from amidoximes and substituted arylboronic acids using DMF as a solvent and employing PTSA as a catalyst. The details will be presented in detail.

Key words : oxadiazaboroles, amidoximes, aryl boronic acids, methodology



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P-67

Allopathic & Ayurvedic

Khushbu A. Patel, Arpi K. Patel, Tarun M. Patel

Kadi sarva vishwavidyalaya

Abstract: medicines are any substance that are ment to change the way your body deals with an illness or injury or to maintain your health and wellbeing. Many types of allopathic medicines are available in market. Allopathic medicines are good and bad according to their use. Ayurvedic medicine must be used more than allopathic medicines. Ayurvedic medicines are available from neature and it has less side effects.

P-68

Nd_2O_3 –Promoted multi-component rapid reaction for the synthesis of 4*H*-pyrans

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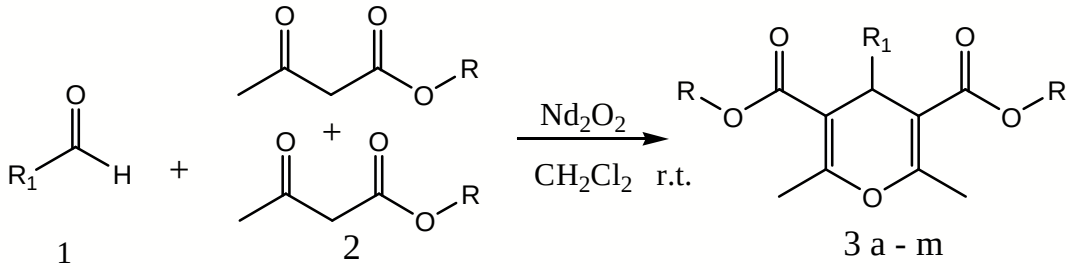
Abstract: The environmental acceptability of the process is improved if the multi-component strategy is applied. Indeed, it is well known that multi-component reactions (MCRs), consisting of two or more synthetic steps, which are carried out without isolation of any intermediate, allow to reduce time, save money, energy and raw materials Hudlicky T. [1]. Moreover, MCRs have the additional advantage of simplicity and synthetic efficiency emerging as an powerful tool in modern synthetic organic chemistry Lavilla et al.[2].

Derivatives of 4*H*-pyran are natural organic compounds with numerous biological and pharmacological activities, such as anti-coagulant, spasmolytic, anticancer, antibacterial, antifungal and diuretic Kreddan et al.[3]. Different synthetic approaches have been reported in the literature for the synthesis of 4*H*-pyran derivatives, including the Michael addiction reaction in α,β-unsaturated dicarbonyl compounds followed by cyclization, [4+2] cycloaddition of enones and alkynes, and multi-component reactions among aldehydes and different active methylene compounds[5]. Recently, these compounds are prepared by condensation of dicarbonyl compounds with aldehydes using $NbCl_5$ as a catalyst over long reaction time Luiz da. et al.[4]



Scheme 1

Herein, we report Nd_2O_3 as a new catalyst for the rapid synthesis of 4*H*-pyrans. Mild reaction conditions, very short reaction time, simple work up procedure and excellent yield of products are the advantages of present protocol.

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P-69

Nd_2O_3 –Promoted one-pot synthesis 2,4,6- triarylpyridine derivatives in aqueous medium

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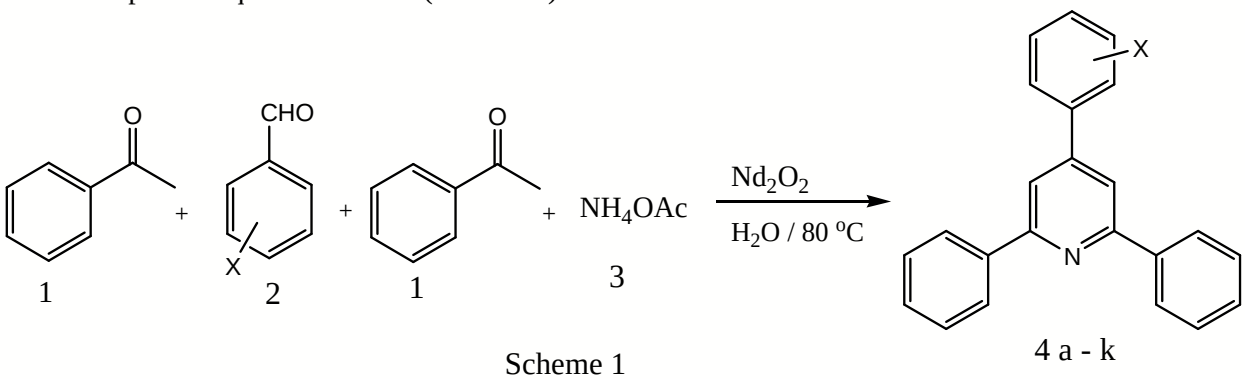
Abstract : Compounds containing pyridine ring system are of great interest because of their pharmaceutical properties such as anticonvulsants, anti-malarial, vasodilator, anti-epileptics and anesthetics Corry et al., [1]. Due to their π-staking systems, triarylpyridines are used as building blocks in supramolecular chemistry Jetti et al.[2]. Conventionally, 2,4,6-triarylpyridine derivatives have been synthesized by condensation of N-phenacylpyridinium salts with α, β-unsaturated ketones in the presence of NH_4OAc Kröhnke et al. [3]. Recently, many improved methods have been reported for the synthesis of these derivatives. However, many of these methodologies suffer from drawbacks such as undesired side products, hash reagents, long reaction time and tedious workup procedures.

In continuation of our efforts to investigate the catalytic activity of Nd_2O_3 for organic transformations, a one-pot condensation of various aldehydes, ammonium acetate and acetophenone have been attempted in aqueous medium (Scheme 1).



Scheme 1

Mild reaction conditions, very short reaction time, simple work up procedure and excellent yield of products are the advantages of present protocol. The investigation of microbial activities of newly synthesized derivatives is in progress in our laboratory.

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P-70

Synthesis of new 2,4,5-trisubstituted imidazole derivatives using copper sulphate as a catalyst under solvent-free conditions

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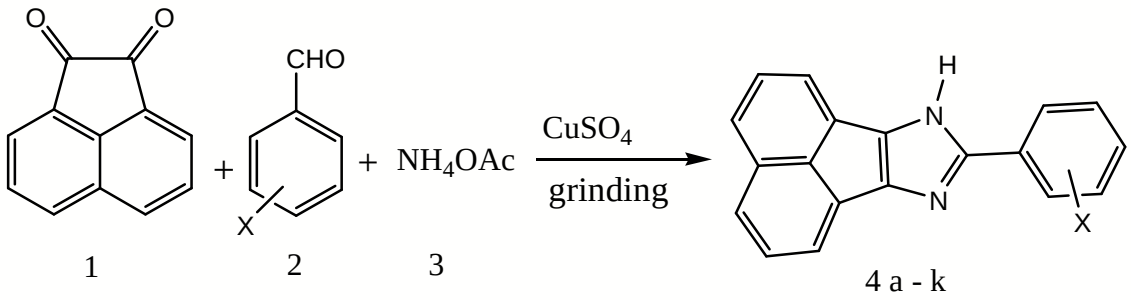
The development of a simple, efficient and general synthetic method for widely used organic compounds from readily available reagents is one of the major challenges in organic synthesis. .In 1858 Debus et al.[1] reported the reaction between glyoxal and ammonia, a reaction that pioneered a novel synthetic route to imidazole. The biological properties of substituted imidazole constitute a significant part of modern heterocyclic chemistry, Grimmet M.R et al.[2].

Exhaustive literature survey indicated that, there are several methods for the synthesis of imidazoles. Many of these reported protocols suffer from one or more disadvantages such as harsh reaction conditions, poor yields, long reaction time, use of hazardous and often expensive acid catalysts. Moreover, the synthesis of these heterocyclic have been usually carried out in polar solvents such as ethanol, methanol, acetic acid, DMF and DMSO leading to complex isolation and recovery procedures.



Scheme 1

Organic reactions were found to occur efficiently and selectively on the surface of solids Toda F [3]. Recently, copper sulphate ($CuSO_4.5H_2O$) has been used as a Lewis acid catalyst for various organic transformations Liao et al [4]. It is an inexpensive, commercially available inorganic solid, soluble in water and extremely safe reagent to be used in chemical reactions. In this communication, we wish to report a simple and efficient one-pot three component solvent-free method for the synthesis of imidazole derivatives using copper sulphate as Lewis acid catalyst (Scheme 1).

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P-71

ZnO Nanopowder catalyzed efficient and convenient synthesis of thiol esters under solvent-free condition at room temperature

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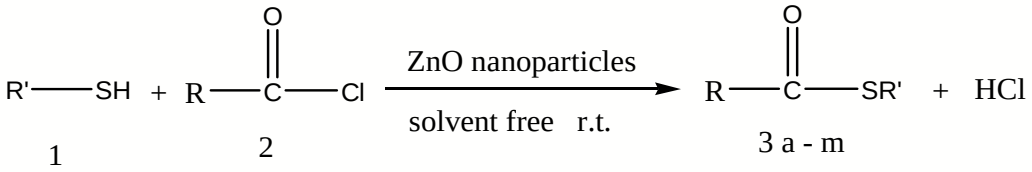
Abstract: Thiol esters are used in the formation of carbon–carbon bonds and other functionalities. In addition, they show higher reactivity and selectivity towards nucleophiles than the corresponding oxygen analogue, which makes them the universal acylation reagents in biochemical processes. These compounds were traditionally synthesized from the reaction of carboxylic acids and thiols Pelter et al.[1]. These methods essentially required activation of acids. A variety of activating agents such as trisalkylthioborane, phenyldichlorophosphonste, tri-n-butylphosphine, diethylphosphorocyanidate, triphenylphosphine N-bromosuccinimide /N-iodosuccinimide and phosgene have been reported for this purpose Cohen et al. [2].

In recent years, zinc oxide has gained much interest in the synthesis of nitriles from aldoximes, the Beckmann rearrangement, Friedel–Crafts acylation More et al. [3] and the acylation of alcohols, phenols, and amines. Recently, zinc oxide nano powder has been used as a catalyst for the synthesis of triaryl pyridine derivatives Reza M. et al.[4]. Herein, we describe a new, simple, and effective procedure for the synthesis of thiol esters from acid chlorides and thiols using zinc oxide nanopowder as a heterogeneous catalyst under solvent-free condition (Scheme 1).



Scheme 1

The advantages of this environmentally benign and efficient protocol include: simple reaction set-up, no need to activate the catalyst, mild reaction conditions, excellent yields of products, short reaction times, and high chemoselectivity.

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P-72

Aroyl Group Driven [1,2] Phosphonate-Phosphate/Phosphine oxide-Phosphinate Rearrangement

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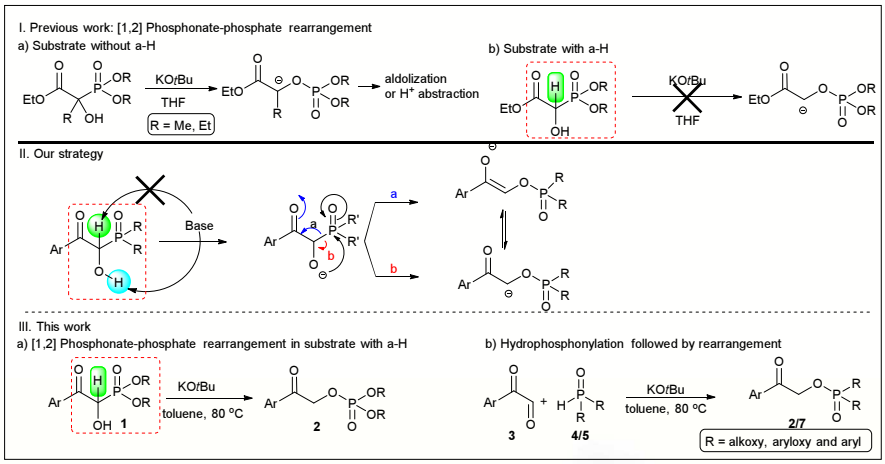
The 1,2-Brook rearrangement is an intramolecular 1,2-anionic migration of organosilyl group from carbon to oxygen in the presence of base.[1] Analogous to this well-studied rearrangement, Phospha-Brook rearrangement is comparatively not well explored.[2] Even though, there are few reports on 1,2-phosphonate-phosphate rearrangement,[3] the influence of functional groups on the migratory aptitude of phospha group over a range of homologous is not well understood. Recently, Johnson and group established base catalyzed direct aldolization of α-alkyl-α-hydroxy trialkyl phosphonoacetates.[3a] This method enlightened a direct glycolate aldolization reaction under basic environment that relied upon the strategic use of [1, 2] phosphonate-phosphate rearrangement (Scheme 1, Ia). However, it limited its application over substrates having α-H. (Scheme 1, Ib). In this regard, we designed a strategy to check if the substrates with aroyl group adjacent to α-carbon can overcome the limitation due to its resonance capability (Scheme 1, II). We were successful in developing an aroyl group driven phosphonate-phosphate rearrangement in dialkyl/aryl(α-hydroxy-β-oxo-β-arylethyl)phosphonates having α-proton under basic conditions and extended to a novel one-pot direct coupling method between 2-oxoaldehydes (2OA) and H-phosphonates/diphenylphosphine oxide.



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P-73

THEORETICAL STUDIES ON SOME METAL NITRIDES AS POTENTIAL HYDROGEN STORAGE MATERIALS, USING DENSITY FUNCTIONAL THEORY

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Abstract : Theoretical studies on hydrogen adsorption were performed on some metals nitrides such as Li_2N_4, Na_2N_4 and K_2N_4 using B3LYP level of theory. Our results reveal that doping of alkali-metal atoms on the nitride systems increases their hydrogen adsorption ability due to electron transfer from the metal atom to the nitrogen surface. The charged surface created around the metal atom is found to enhance the hydrogen adsorption capacity of the complex from 9 to 16.79 wt% with an average binding energy of 0.30 for Li_2N_4, 0.06 for K_2N_4 and 0.07eV/H_2 in case of Na_2N_4 . Various Conceptual density functional theory based global and local reactivity descriptors, were used for this purpose. We have also calculated the dependence of the Gibbs free energy change (ΔG) of H_2 adsorption process at various temperatures. The complex shows an increase in the kinetic stability with the successive addition of H_2 molecules.

Keywords : Metal nitrides; Conceptual reactivity descriptors; Physisorption

P-74

Air-Assisted 2-oxo driven Dehydrogenative α,α-Diamination of 2-oxoaldehydes to 2-oxoacetamidines.

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Air assisted, functional group driven, mild, additive free, three-component synthetic approach to different 2-oxoacetamidines from 2-oxoaldehydes, secondary amines, and anilines was successfully developed. Mechanistically, the transformation is through a highly unstable system (RCOCHN1N2) that rearranges at room temperature and undergoes air assisted dehydrogenation to different 2-oxoacetamidines. Since, amidines are well known structural motifs present in numerous bioactive natural products, pharmacophores, synthetic intermediates, and also act as efficient coordinating ligands,[1] the synthesis of 2-oxoacetamidines in particular employing milder method is desirable. The traditional synthesis of 2-oxoacetamidines, in general, rely on metal-catalyzed coupling reactions.[2] These methods as evident involve metal salts, required expensive substrates or were produced in more than one step, had limited substrate scope, and as a result lead us to think about developing alternative chemistry.

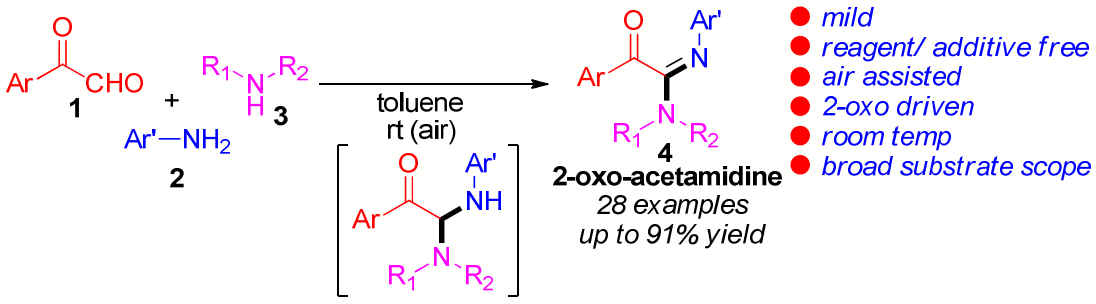

Figure 1: Summary of our work

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P-75

Allopathic & types

Yash h. chaudhari, Sachin m. patel, Tarun m. Patel

Kadisarva vishwavidyalaya

Abstract: Medicines help us to get better when we are unwell Medicines are any substance that are meant to change the way your body deals with an illness or injury or to maintain your health and wellbeing. Drugs are made into various dosage forms so that they can be easily administered or can be delivered to the right part of the body. Some of these medicines are available in other stores and market.

P-76

Nature Inspired Hydrogel Based Wound Patch Infused with Antimicrobial and Antioxidant Agents for Accelerated Wound Healing

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A one-pot preparation of hydrogel based wound patch having antimicrobial silver NPs (Ag NPs) and antioxidant Epigallactocatechin gallate (EGCG) was developed for scar free quick wound healing. As a precursor to hydrogel synthesis, natural polymer Guar Gum (GG) was modified to obtain cationic surface charges (AGG) which were utilized for *in-situ* reduction of silver salt to Ag NPs besides Ionotropic Geletion with anionic alginate. The composition of hydrogel wound patch was fine tuned stoichiometrically apropos supportive ingredients to obtain the desired attributes for the wound patch. Synthesized hydrogel and its precursors were fully characterized and their physico-chemical, mechanical and biological properties were assayed. The bio-efficacy of the wound patch against fibroblast cells and microbes was also studied. Interestingly, the various components *viz* AGG, Ag NPs (antimicrobial), EGCG (radical scavenging) exerted their effects, concomitantly stimulating fibroblast cells growth and proliferation. Meanwhile, these samples showed appropriate tensile strength, porosity and swelling ability for absorbing wound exudates. The clinical applicability of the wound patch was validated *in vivo* using Wistar rat as a model. The progression of wound healing was compared with commercial available wound patches. Preliminary observations point out the designed hydrogel patch accelerated the healing process with better wound contraction, promoted collagen deposition and enhanced vascularization of wounded region. These initial results of *in vitro* and *in vivo* assays substantiate the possible clinical application of designed wound patch for accelerated wound healing. Detailed analyses of bio-molecular parameters are underway.

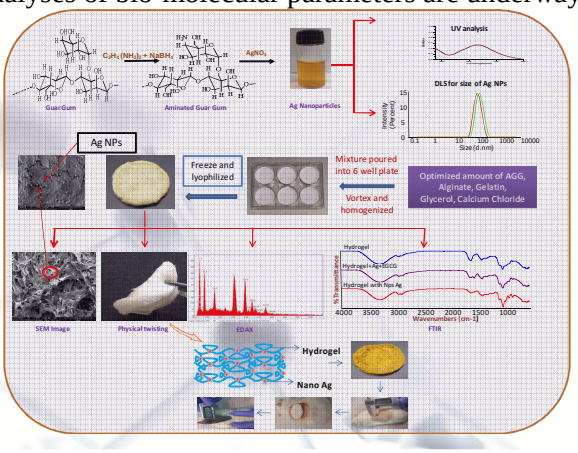

Fig.- Graphical Representation of abstract

P-77

Diversity of folds in venomous *Conus* peptide toxins

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Conopeptides are small peptides isolated from the venom of marine molluscs of the genus Conus and have long held the interest of biologists, pharmacologists, and structural biologists. Conotoxins are small disulfide-rich peptides from the venoms of marine cone snails. They target a variety of ion channels, transporters, and receptors and are of much interest as drug leads [1]. Conotoxins bind diverse targets with high specificity as a result of their well defined structures and high structural diversity. This structural diversity is the focus of our study [2].

To appreciate the structural diversity of conotoxins, it is necessary to appreciate their vast sequence diversity. Although conotoxins are generally restricted to 10-40 residues and the majority contains two or three disulfide bonds, there is still considerable scope for sequence variation, disulfide framework variation, and additional complexity introduced by the large number of post-translational modifications that are characteristic of the conopeptide family [3].

In the present study, we have analysed structural features of conotoxins in the context of its functions. Correlations were made between cysteine pattern, disulfide connectivity, and secondary structural features of the conotoxins. We have also attempted to compare the structural features of conotoxins with other venomous peptide toxins. Analysis of co-crystal structures of conotoxins with channel/receptors has facilitated to shade more light on advantage of conotoxins to use as a bioavailable peptidic drugs.

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P-78

Cu(II)-Mediated *ortho*-C−H amination/thiolation of Arenes and Heteroarenes

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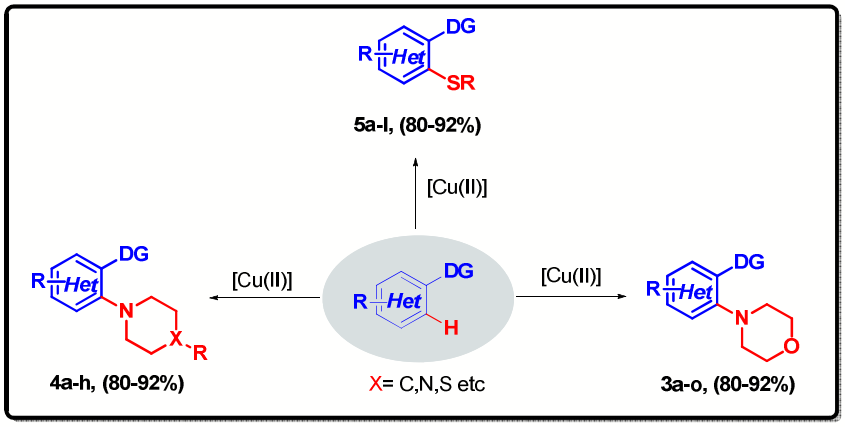
In the recent year, the C-H activation have been emerged as a powerful strategy for the construction of complex molecules due to its high step- and atom-economy as well as the readily accessible starting materials.[1,2]We have design adirecting group assisted protocol for the C-H amination/thiolation of arenes and heteroarenes under mild reaction condition. No additive was required in the reaction. By this method, the secondary amine (e.g; piperazine, piperdine and pyrrolidine) could be incorporateddirectly at *ortho*position of arenes/heteroarenes.The new compounds have been fully characterized by spectroscopic, spectrometric and X-ray crystallographic analysis. We further perform deuterium labelling experiment to explain mechanism of the reaction.



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P-79

An Efficient Route for Synthesis of Tetrahydro-Pyridocarbazoles from *o*-Alkynylaldehydes *via* Decarboxylative Cyclization/Ring Expansion

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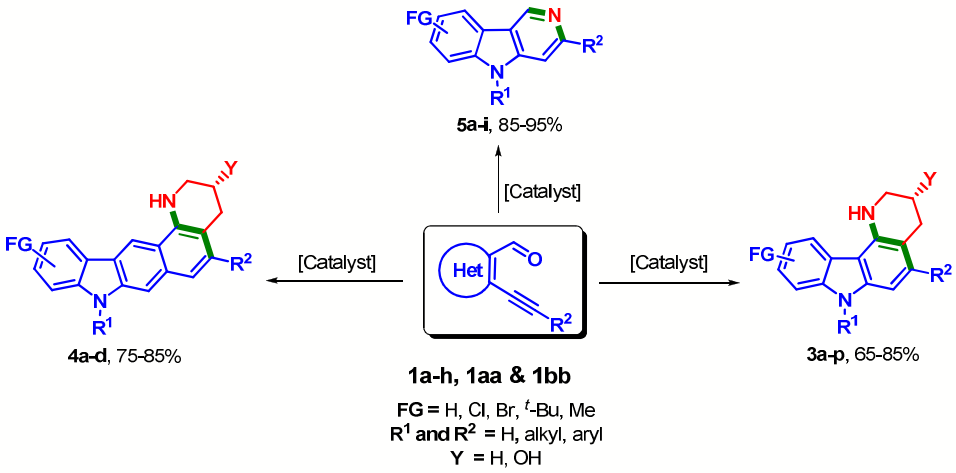
In the continuation of our ongoing lab work using *ortho*-alkynylaldehydes, [1,2] we have design an efficient approach towards synthesis of highly diversified 5-aryl-2,3,4,7-tetrahydro-1*H*-pyrido[3,2-*c*]carbazole 3, 5-aryl-2,3,4,8-tetrahydro-1*H*-quinolino[7,8-*b*]carbazole 4 and carboline 5 derivatives utilizing decarboxylative cyclization and ring expansion has been developed. The secondary α-aminoacids reacts with 2-alkynylaldehyde to form an azomethine. Subsequent decarboxylation, cyclization and ring expansion of azomethine provides heteroatom or nitrogen containing 6-membered ring. By virtue of this expedient method, a series of heteroannulated carbazoles can be synthesized efficiently. The X-ray crystallographic studies supported the proposed mechanistic pathway for the targeted cyclized product.



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P-80

Radical–Radical Cross Coupling Reactions of Photo-Excited Fluorenones

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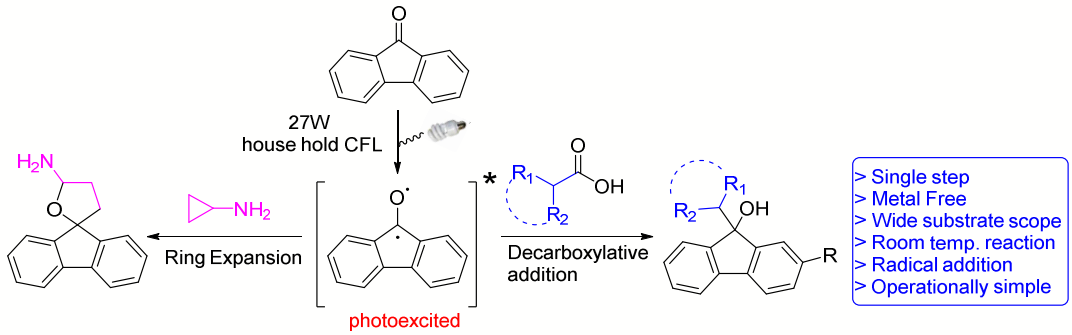
Photoredox reactions involving ketyl radicals have recently found applications in intra or inter molecular cyclization,[1] self dimerization of aldehydes or ketones, [2] reductive epoxide/aziridine ring opening [3]and asymmetric ketyl/α-amine radical coupling reactions. [4] However, the generation of ketyl radicals still poses a great challenge owing to unfavorable activation barriers during their preparation. The activation barrier further increases in the case of ketones, thereby limiting potential applications to aldehydes only. Radical–radical cross coupling reactions of photoexcited 9-fluorenones have been accomplished for the first time, leading to the synthesis of 9-alkyl, pyrollidinyl and spiro-THF derivatives of 9-fluorenones. The method also reveals, for the first time, the behaviour of ketyl radicals in decarboxyaltive alkylation and ring expansion reactions. The method showcases a dual role of 9-fluorenoneviz., one its ability to generate ketyl radical and second to undergo free radical cross coupling. Notably, this is also a first report involving use of acids as traceless activation groups in the presence of 9-fluorenone, although several reports have appeared utilizing them for alkynylation, cyclization and cross-coupling reactions [5]. we present the first radical cross coupling reactions of 9-fluorenones leading to the synthesis of 9-alkyl, pyrollidinyl and spiro-THF derivatives of 9-fluorenones. Moreover, the reaction shows for the first time propensity of ketyl radicals to participate in decarboxyaltive alkylation and ring expansion reactions. Furthermore, the method is metal free, operational simple, requires no elaborate setup and has wide substrate scope.



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P-81

Synthesis of Amides and Azobenzenes via Aminyl Radical Cation Catalysed by Cu-Mn Spinel Oxide

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Abstract: A highly efficient Cu-Mn catalyzed process for the aminolysis of esters has been developed. Also, the catalyst promotes self as well as cross dehydrogenative coupling in anilines to generate symmetric and unsymmetrical azobenzenes respectively. The method employs neutral conditions, inexpensive catalyst, high yields and wide functional group tolerance. Unarguably amide linkage represents one of the most commonly executed transformation in synthetic as well as medicinal chemistry programmes owing to its pervasive presence in diverse biological systems like proteins, natural products and pharmaceuticals.[1] The synthesis of amides is generally achieved via coupling of carboxylic acids with amines.[2] However, it suffers from drawbacks such as generation of side product formation and dry reaction conditions. This has shifted attention of reserchers towards finding alternative substrates such as aldehdyes, alcohols and halides for direct amidation with amines. [3] The drawback with conventional amidation of esters is use of excess of base and very few catalytic approaches are known to address this issue. [4]

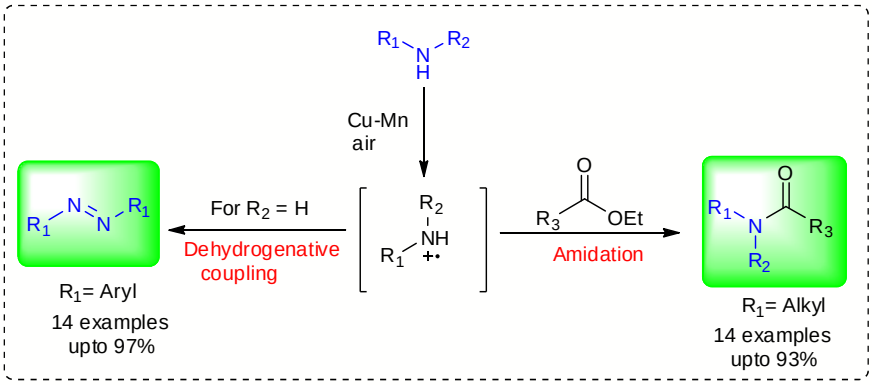

Figure 1: Summary of our work

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P-82

Photoredox-Catalyzed Radical Addition of Thiols to Synthesise Highly Diastereoselective 3,4-Di-substituted γ-Lactones

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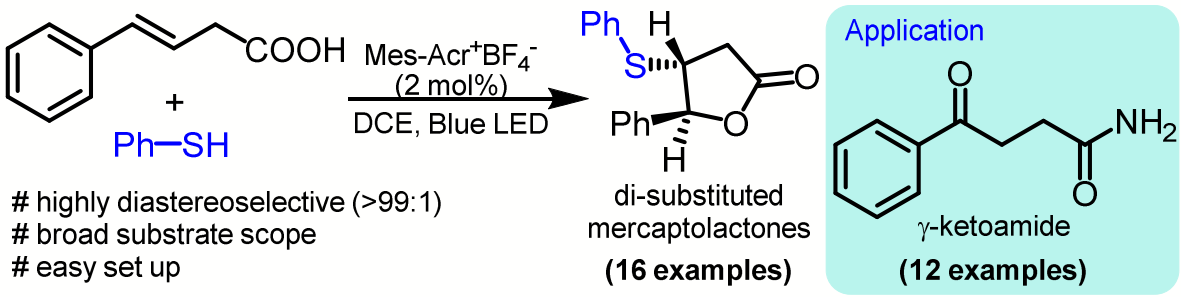
Abstract: Herein, we report a first visible light mediated radical addition of thiols on 4-phenylbut-3-enoic acids to give highly diastereoselective synthesis of 3,4-disubstituted γ-lactones (>99:1). The reaction precludes the conventional prerequisite of conjugate addition. Furthermore, the lactones were successfully utilized in the synthesis of γ-ketoamides, a privileged structural motif. Sulfur-containing compounds comprised as much as one-fifth of the 200 most-prescribed pharmaceutical products in 2011.[1] The classic way to introduce a sulfur group on an alkene is via Michael addition,[2] which makes their addition on the non-conjugated system challenging. In this regard, thiyl radicals easily obtainable from corresponding thiols or disulfides can trigger a diverse range of reactions like thiol-ene coupling reactions, addition of thiols to alkynes, the addition of sulfonyl chlorides, decarboxylative additions of amino-acids via Giese reaction, thiol-ene reactions, photo-oxygenation, inter-molecular cyclizations, addition of alkyl halides and atom transfer reactions.[3]



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P-83

Controlled Release of Insecticide Using Eco-Affable Cenospheres-Alginate Microbeads

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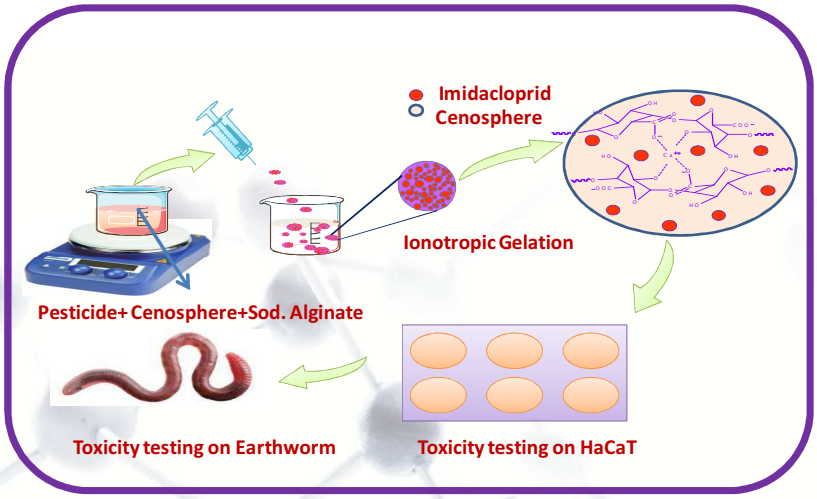
ABSTRACT: Global demand has ushered an increased yield in crop around the world with improved seeds and crops, increased use of fertilizers and pesticides, new farming technologies, and advanced agricultural machinery. Accelerated use of pesticides in boosting agriculture instigated us to explore smart release formulations to taper the consumption of these unsound chemicals. Polymeric beads of alginate and cenospheres, impregnated with an insecticide, **Imidacloprid** were developed through ionotropic gelation. The aim was to improve upon the limitations of the conventional agrarian practices through novel interventions towards sustainable agriculture. High pesticide loading of 64% was achieved at the alginate and cenosphere ratio of 1:3 with a loading feed 1:10, of **Imidacloprid** and Cn-Alg stoichiometrically and at the crosslinker concentraton 0.25M. The physico-chemical attributes of Cn-Alg microbeads were confirmed by ATR-FTIR, SEM, EDX, TGA and BET techniques. The results reveal an insight into the functional groups, size, texture, elemental composition, thermal stability, and surface area. The entrapment and release of **Imidacloprid** were determined by UV-Vis. Further, release studies revealed the delayed release of the **Imidacloprid** in all the formulations of Cn-Alg compared to bulk **Imidacloprid**. The pesticide microbeads will be evaluated for its toxicity on human skin cell line HaCaT and on earthworm, one of the non-target organisms (as per OECD guidelines), to assess any risk involved in the occupational exposure during its application and to gauge any alteration in the environmental footprint of farming. The present work embodies better pest control and crop management utilizing a waste product from one source towards sustainable eco-farming.

Keywords: Alginate, Cenospheres, Imidacloprid, Encapsulation, Microbeads.



P-84

Synthesis of Reverse Building blocks of Milk Oligosaccharides

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The growing significance of oligosaccharides as constituent biologically important compound has a sparked considerable interest of chemist for their synthesis. Amongst the various oligosaccharide isolated from different sources, the milk oligosaccharide has emerged as important biologically active compounds. It has been seen that the milk oligosaccharides are comprised of various core-units and every core-units has lactose at its reducing end, besides that the milk oligosaccharides contain glucose, galactose, GlcNAc, GalNAc, fucose and sialic acid at its non-reducing end. The presence of these mono-saccharides and the position of glycosidic linkages play a definite role in their biological activity. Various building blocks of milk oligosaccharides have been synthesized by different workers in which the lactose was present at the reducing end. In this present paper we have synthesized the **reverse building blocks** of milk oligosaccharide meaning thereby in the trisaccharide which we are reporting here, contain the lactose at its non-reducing end. The monosaccharide units which we have selected for the trisaccharide building blocks are glucose and fucose. For this purpose we have synthesized the lactose as a donor as its trichloro acetamidate and simultaneously the acceptors of glucose and fucose were also been synthesized and glycosidation of these acceptors and donor has been made successfully by TMSOTf method, which results in the formation of four trisaccharides namely- **Methyl-2-O.-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl(1→4)-2,3,6-tri-O-acetyl-β-D-glucopyranosyl)-3,4-O-isopropylidene -α-L-fucopyranoside (a), Methyl 3-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl-(1→4)-2,3,6-tri-O-acetyl-β-D-glucopyranosyl)-2,4-di-O-acetyl-α-L-fucopyranoside (b), Methyl-4-O-(2,3,4,6–tetra –O-acetyl-β-D-Galactopyranosyl(1→4)-(2,3, 6 tri –O-Acetyl- β -D-glucopyranosyl)-2,3-di-O-acetyl-6-O-benzyl-α–D-glucopyranoside(c) and Methyl-4-O-(2,3,4,6–tetra –O-acetyl -β-D- Galctopyranosyl(1→4)-(2,3,6-tri–O-Acetyl-β-D-glucopyranosyl)-2,3,4-tri-O-acetyl-α–D-glucopyranoside(d).** The structures of synthesized trisaccharides were confirmed by NMR spectroscopy.

Key words: Milk oligosaccharides and reverse building blocks.

P-85

Hierarchically porous sphere like copper oxide (HS-CuO) Nanoparticles catalysed synthesis of Imidazo[1,2-a]pyrimidine derivatives.

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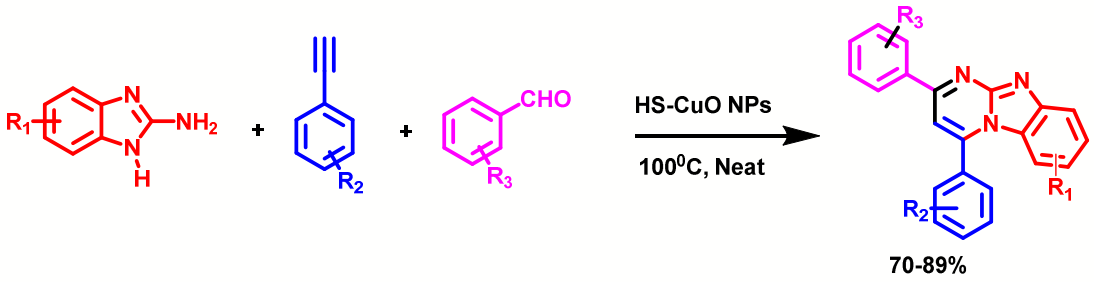
Abstract: Imidazo[1,2-a]pyrimidine moiety is an important pharmacophore found in various biologically active molecules which shows antimicrobial, anticancer, antitubercular and antifungal activities.[1] Most of the known method of the synthesis of imidazo[1,2-a]pyrimidine involves multistep synthetic protocol, longer reaction time and use of non-recyclable catalytic system and additives. To overcome these limitation and in continuation of our interest towards nanocatalysis,[2-5] we propose an alternative eco-friendly synthetic methodology for the synthesis of imidazo[1,2-a]pyrimidine using hierarchically porous sphere like copper oxide (HS-CuO) nanoparticlesas a catalytic system.[6] For achievement of sustainable chemistry, nanocatalysis plays significant role with several advantages like more exposedsurface area, recovery and recyclability of catalyst with less waste generation.[7] This method is efficient due to recyclability of nanoparticles without loss of its activity, avoid usage of additives or bases and showed ideal values of green chemistry metrics such as low E-factor, high atom economy, process mass intensity (PMI), reaction mass efficiency (RME) and carbon efficiency (CE).



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P-86

Novel one-pot synthesis of 2-pyrimidinaminecore derivatives via green chemistry approach and their larvicidal activity

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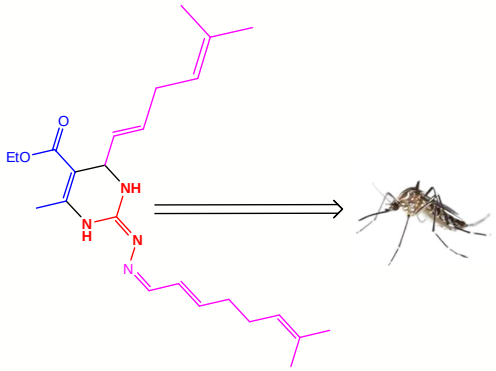
Culex is an important mosquito vectors for the transmission of serious diseases, such as filariasis, West Nile virus, dengue, yellow fever, chikungunya and other encephalitides. Nearly one billion people in the developing countries are at risk. In order to discover new bioactive molecules and pesticides acting on mosquito, we designed active amide structure and synthesized a series of novel pyrimidine derivatives. A series of novel pyrimidine derivatives were characterized by FTIR, ^{1}H NMR, ^{13}C NMR, and HRMS. The single crystal structure of compound was determined to further elucidate the structure. Biological activities of these compounds were tested. Most of them exhibited higher mosquito larvicidal activity. Especially some of displayed relatively good activity to reach 92% at 2 µg/mL. Therefore,2-pyrimidinaminesynthesis was carryout via the reaction involved for amine with pyrimidine interaction. This study suggests that the 2-pyrimidinaminederivatives exhibited good effective against mosquito.



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P-87

Synthesis and spectroscopic properties of *β,β'*-fused pyridoporphyrins.

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ABSTRACT: Porphyrins are important class of π-conjugated heterocycles which have great deal of attention due to their potential applications in diverse areas including medicine, catalysis, material science, biomimetic models for photosynthesis, organic light emitting diodes, near infrared dyes, hybrid solar cells, biosensors and as photosensitizers in photodynamic therapy applications.[] The incorporation of π-conjugated system at the periphery of porphyrins modify their electronic properties and hence show a significant bathochromic shift in their UV-Vis spectra. For efficient electron transfer,[] large two photon absorptions [] and light harvesting [-] characteristics, a large number of chromophores have been attached on the periphery of porphyrins. Among these, the *β,β'*-fused porphyrins have achieved a great deal of attention in the past few years. Therefore, we were interested to develop an efficient strategy to synthesisze *β,β'*-fused pyridoporphyrins in appreciable yields. The details related to the synthesis, spectroscopic characterization and electronic properties of these newly synthesized macrocycles will be presented.

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P-88

Temperature Dependent Empirical Polarity Parameters of Solvate Ionic Liquids

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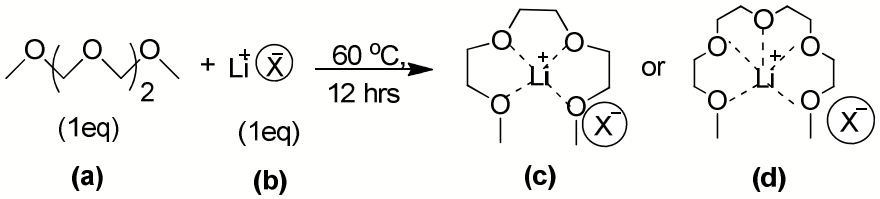
Abstract: Solvate ionic liquids (SILs) are an emerging class of solvents with excellent potential as electrolytes for lithium ion batteries, [1-2] electro-deposition,[3] reaction media, [4] etc. Solvate ionic liquids are formed by mixing equimolar mixture of glyme (oligoether) and alkali metal salts. SILs show properties that are similar to those of conventional ionic liquids such as high ionic conductivities, high viscosities and low vapour pressures but are easier to synthesize.

In order to explore the polarity of SILs, empirical polarity parameters discovered by Catalan such as solvent acidity (SA) , solvent basicity (SB), solvent polarity (SP), solvent polarity polarizability (SPP) and solvent dipolarity (SdP) were determined.[5] To study the temperature effect, the variation in polarity with change in temperature was recorded and analyzed. The polarity parameters provide very rich information about solute-solute, solute-solvent and solvent-solvent interaction in SILs and help to understand the physicochemical properties of SILs.

Scheme:



a = G_3 (Triglyme) / G_4 (Tetraglyme)
b = Li[NTF_2] /Li[OTf]

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P-89

Synthesis and photophysical properties of *β,β'*-fused benzo[f]quinoxalinoporphyrins

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ABSTRACT: Porphyrins are important class of conjugated macrocycles which have demonstrated several applications in various scientific fields such as medicine[1], supramolecular chemistry[2], catalysis[3] and also play a central role in natural processes including photosynthesis and oxygen transport[4]. The conjugation of π-electrons in these molecules can be extended through peripheral functionalizion of porphyrins. To this end, we have developed a simple and efficient method for the synthesis of a new series of π-extended *β,β'*-fused benzo[f]quinoxalinoporphyrins in good yields. The details about the synthesis, spectroscopic characterization and photo physical properties of these newly synthesized *β,β'*-fused benzo[f]quinoxalinoporphyrins will be presented.

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P-90

Guest Dependent Unusual Rigidity of the Flexible Metal-Organic Framework

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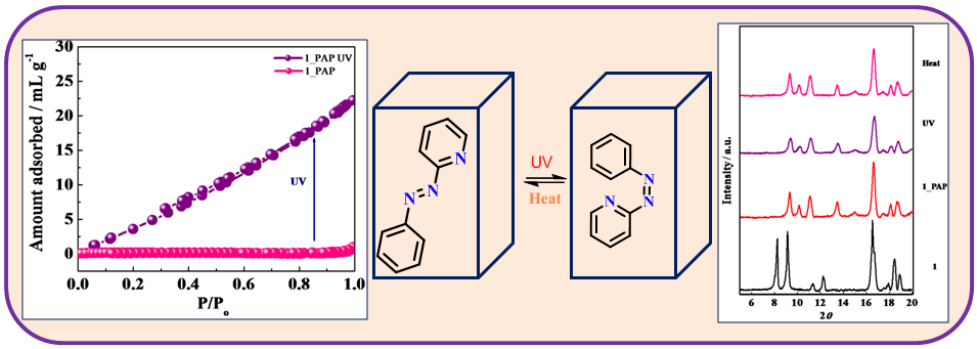
A novel photochromic guest molecule, 2-Phenylazopyridine (PAP) was successfully introduced into a porous metal organic framework, $[Zn_2(terephthalate)_2(triethylenediamine)]_n$ (**1**)[1]. The successful embedment of PAP has been confirmed by elemental analysis, XRPD measurements, IR spectroscopy etc. The number of PAP molecules per unit cell of **1** was 1.0, as evidenced by elemental and thermogravimetric analyses of the host-guest composite, **1**⊃PAP. The composite **1**⊃PAP did not adsorb N_2, revealed by low BET surface area (0.6182 m^2/g) of **1**⊃PAP which indicates the pore blockage by the close contact of the host framework with the guest PAP. The light induced trans/cis isomerization of the guest molecule (PAP) in this flexible hybrid host-guest compound, **1**⊃PAP has been investigated through IR spectroscopy.[2-3] Switching can also be achieved by irradiation with UV light and back-switching using heat with detectable changes although the switching process is partially reversible. Cis/trans isomerization of the guest PAP inside the composite of **1**⊃PAP does not show any structural transformations of the host suggest sustained rigidity of Metal Organic framework, $[Zn_2(terephthalate)_2(triethylenediamine)]_n$ (**1**).



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P-91

Synthesis of Cu-catalysed quinazolinones using a Csp3–H functionalisation/cyclisation strategy

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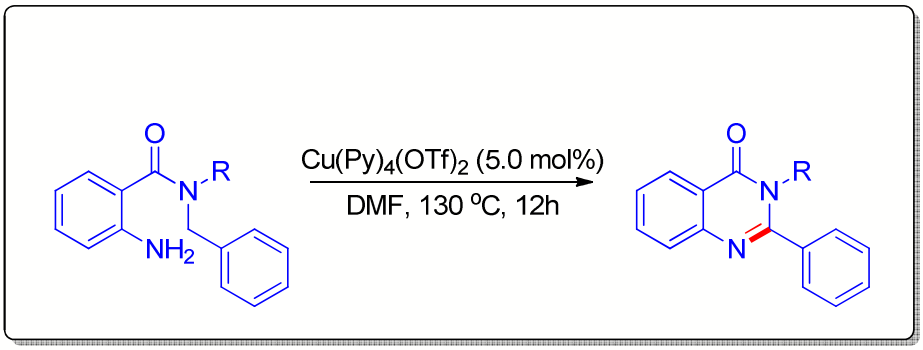
Abstract: C–H bond functionalizationhas been growing at a rapid rate and still has a huge scope for further development and making it more versatile in organic synthesis. Use of easily available and cheaper source of transition metal like Copper in C–H activation is the better alternative for C–H bond functionalization. Through C–H bond activation the synthesis of biologically active compounds like quinazolinone and its derivative can be done very easily.Quinazolinone as well as quinazoline has wide spectrum of biological application from antibacterial, antifungal, anticonvulsant, anti-inflammatory, anti-HIV, to anticancer. There are so many drugs available in market out of which, some contains quinazolinone as core structure of molecule.[1]

In comparison to the reported methods our strategy allows an easy access, to synthesize diverse substituted quinazolinones under mild conditions by using copper catalyst,[2,3,4,5] to develop the protocol for the synthesis of quinazolinone from 2-amino-N,N-dibenzylbezamide. The commercially available Tetrakispyridinecopper(II) bistriflate gives desired quinazolinone in competitive yield under air in DMF solvent.



To determine the mechanism of the reaction, we have added TEMPO into the reaction mixture, under standard reaction conditions, which results the quench of the reaction. This evidence proves the reaction goes through SET mechanism. Again under N_2 atmosphere the yield of the reaction decreases almost four times, indicates that molecular oxygen also plays an important role in reaction mechanism.

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P-92

Dehydrozingerone: Synthesis of alkyne-azide cycloaddition analogues and their anti-cancer activity

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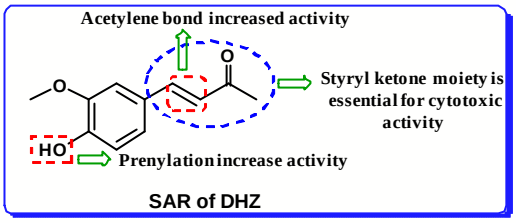
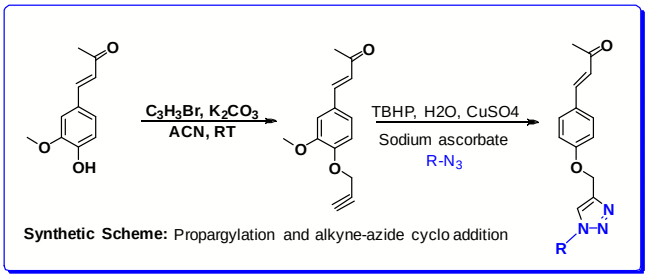
Dehydrozingerone(DHZ) is isolated from rhizomes of ginger (*Zingiber officinale*) [1]. DHZ, which is a recognized biosynthetic intermediate and degradant of curcumin [3][4], possesses the structural resemblance with curcumin, as both bear styryl ketone moieties with similar substitutions on the phenyl ring [5]. DHZ has shown significant therapeutic potential with profound biological properties, such as anti-inflammatory, antioxidant, antifungal and anti-mycobacterial activity]. Herein, we report the isolation and synthetic modification of Dehydrozingerone. We synthesized the *O*-propargylated Dehydrozingerone which was subsequently coupled by alkyne–azide cycloaddition using click chemistry. The synthesized compounds were evaluated for their *in-vitro* cytotoxic activity in a panel of three cancer cell lines. Some of the synthesized molecules displayed a potent cytotoxic potential with IC_{50} value ranging from 1.8-3.0 µM in MCF-7, PC-3 and HCT-116 cell lines. Further, the compounds showing cytotoxic potential in all the cell lines tested, demonstrated a significant anti-invasive potential in prostate cancer cells. The mechanistic study of these compounds showed that they not only suppressed the AKT/mTOR signalling which regulates nuclear transcription factor-NF-kB, but also augmented the expression of anti-invasive markers E-cadherin and TIMP. These compounds significantly declined the expression of pro-invasive markers Vimentin, MMP-2 and MMP-9 respectively. Taken together, this study underscores an efficient synthetic approach employed to evaluate the structure activity relationship of Dehydrozingerone in search of potential new anticancer agents.





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P-93

Studies on Bioactivity of some Schiff Base Complexes of Cu(II), Ni (II) and Zn (II).

Nusrat Shafi, Majida Maqbool

A Schiff Base resulting from the interaction of cinnamaldehyde with p-anisidine forms tetradentate complexes with Cu (II), Ni (II), and Zn (II). Elemental analysis, molar conductance, magnetic susceptibility, IR, UV-Vis and ^{1}HNMR studies of the Schiff Base and its Complexes have been carried out and the structure of the complexes have been determined from the data. It is found that the geometry of the complexes is square-planar. All the resulting complexes were screened for antimicrobial activity by the well diffusion technique using DMSO as the solvent at 36^{o} C and for a period of 18 to 21 Hrs.The minimum inhibitory concentration (MIC) values were calculated. All the complexes have been found to be antimicrobially active and show higher activity than the free ligand.

P-94

Novel Water-Soluble Phosphatriazenes: Ligands for Copper-Free Sonogashira and Column-Free Suzuki Coupling of Nucleosides

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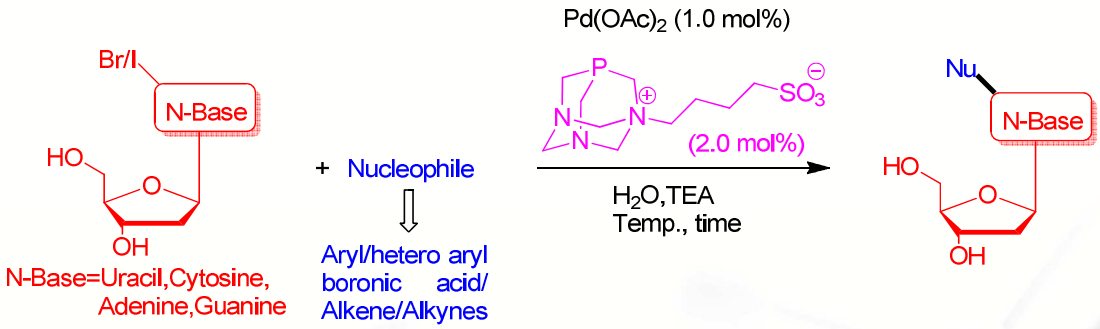
Abstract: Palladium catalyzed cross-coupling reactions are a powerful method to attach carbon or heteroatom groups to the heterocyclic baseas these modified molecules show high biological activity and high fluorescence[1]. These modifications of nucleosides have been demonstrated reliably using palladium-catalysed cross-coupling reactions by several research groups along with their applications [2]. However, they have used high loading of palladium, copper (I) salt as co-catalyst (for Sonogashira reaction), non-aqueous solvents, and column chromatography for purification, which are not environment friendly.Hence it makes the synthetic procedure less striking[3]. So, we have synthesized two new water soluble Phosphatriazenes ligands. Spectroscopic techniques (^{1}H, ^{13}C, ^{31}P, FTIR etc.) and structural characterisation by X-ray diffraction of ligand confirmed the proposed structure.

The new ligand with $Pd(OAc)_2$ exposed as excellent catalysts for environment friendly, highly efficient Suzuki-Miyaura cross-coupling of (hetero)aryl boronic acid in water. The water-solubility of the catalytic system simplified the isolation of the cross-coupled products to mere filtration, while the catalytically active solution in the filtrate was recycled eight times. A novel copper-free Sonogashira coupling protocol for the nucleosides has also been established via a one-pot synthesis of FV-100, a nucleoside based drug in phase 3 clinical trials for herpes zoster or shingles treatment. Application of the Heck reaction was demonstrated by the synthesis of another antiviral drug: BVDU.



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P-95

Apoptotic and anti-metastatic activity of ethanolic leaf extract of an Indian medicinal plant in human non-small cell lung cancer A549 cells

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Medicinal plants have vital role in the history of mankind especially in the field of medicine. India is very rich in medicinal plants and different parts of plants have long been used in ayurvedic medicine for the treatment of several complex disorders including cancer. Here we investigated apoptotic and anti-metastatic property of crude ethanolic extract of leaf from an Indian medicinal plant which is rarely explored for its anti-cancer activity.

A549 cells were treated with different concentrations (0-600 µg/ml) of ethanolic extract of leaf for 24 hrs to investigate pathways of induction of apoptosis and anti-metastatic property. Cytotoxicity,cell morphology, nuclear fragmentation, cell cycle arrest, mitocondrial membrane potential, Caspase-3 activation were studied to check its apoptotic effect. To investigate anti metastatic activities, we have done wound healing assay, cell migration assay and gelatin-zymography.

We found that crude extract induced apoptosis via intrinsic pathway of apoptosis like loss of mitochondrial membrane potential, caspase-3 activation, cell cycle arrest and apoptotic body formation. Additionally,crude extract also reduced the cell migration and wound healing. Activity of MMP-2 and MMP-9 was decreased significantly after treatment with plant extract (100 µg/ml). Significant apoptosis induction and metastasis inhibition was observed at100 µg/ml.

So, our crude extract induces apoptosis and reduces metastasis in highly metastatic cancer A549 cells. Since our crude extract is effective at as low as100 µg/ml, the active ingredient is possible a great extent to control highly metastatic cancer cells.

P-96

PARP-1 depletion in combination with either High or Low LET radiation reduces the metastatic potential in cultured human cells by suppression of MMP activity

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High LET carbon ion is producing promising clinical results worldwide due to its ability to kill radio-resistant tumor and its anti-metastatic activity. In contrast cells irradiated with low LET gamma rays have been shown to increase the metastatic potential of cancer cells. Poly (ADP-ribose) polymerase-1(PARP-1) inhibitors have been widely used as radiosensitizer and many of them are in clinical trial against various types of cancer. The purpose of this study was to investigate the effect of PARP-1 depletion in combination with either Carbon Ion Beam (CIB) or gamma irradiation on metastatic potential of cultured cancerous cells.

Human cancer cells were treated with PARP-1 inhibitor and irradiated with CIB or Gamma. The irradiated cells (0-4Gy for CIB whereas 0, 2, 4, 6, 10 Gy for gamma) were tested for cell migratory assay and MMP-2 and MMP-9 activity. Alterations of mRNA expression of the MMP-2, MMP-9 genes and in some of the genes those are involved in cell migration were studied.

CIB exposure significantly reduces activity of MMP-2 and MMP-9, which further diminishes when cells were PARP-1 depleted in addition to CIB. On the Contrary, MMP- 2 and MMP-9 activity significantly increases in cells irradiated with gamma, whereas its activity gets reduced upon PARP-1 depletion with gamma in a dose dependant manner. The mRNA expression of the MMP genes and the migratory potential was also found to be down-regulated in a dose dependant manner in CIB irradiated cells with and without PARP-1 depletion. However, MMP expression and migratory ability of the gamma irradiated cells were found reduced only when it is combined with PARP-1 depletion. Thus, our study clearly demonstrates that PARP-1 inhibition in combination with either high or low LET can be a promising tool in controlling metastatic cancers.

P-97

A novel G-quadruplex ligand having intrinsic fluorescence and permeable to cultured human A549 cells.

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G-quadruplex DNA is a special three dimensional structure where backbone of DNA folds to form four-stranded structure and four G from each strand makes hydrogen bond in a plane stacked one above another[1]. There are huge topological variations of G-quadruplex structure which depends on G-tract sequence[2]. G-quadruplex forming sequence is found various positions in human genome especially at the promoter region of different oncogenes and telomeres[3][4]. So, G-quadruplex stabilizing molecules can inhibit oncogenic expression as well as telomerase activity and hence has long been attactive field to produce potential anti-cancer agents[5]. Here we report a novel G-quadruplex ligand obtained from ZINC database after screening by theoritical studies.

We have checked the G-quadruplex binding ability of the compund using standard G4-FID (G-quadruplex Fluorescence Intercalator Displacement) assay[6]. We have treated the A549 cells with different doses of this compound for (0-48 hrs) and did MTT assay to check cell cytotoxicity. We also tested the cell permeability assay.

Thiazole orange (TO) gives intense fluorescence upon binding with G-quadruplex DNA and decrease of such fluorescence in presence of this compound proves its G-quadruplex binding ability in G4-FID assay[6]. We observed better replacement of TO from G-quadruplex (22AG) DNA than calf thymus DNA by this compound. MTT assay shows slight toxicity (30% cell death) to the cells at 50 µM for 48 hrs. This compound has intrinsic fluorescence in visible region and is permeable to cultured human A549 cells. Further studies are going on to check its inhibitory effect on oncogenes and/or telomerase, if any. Fluorescence property of this compound has added advantage to check in vivo localization like in telomere or in promoters of oncogenes by FISH studies.

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P-98

Lewis Acid Catalyzed [3+2] Cycloaddition of Donor- Acceptor Cyclopropanes and 1-Azadienes: Synthesis of Imine Functionalized Cyclopentanes and Pyrrolidine Derivatives

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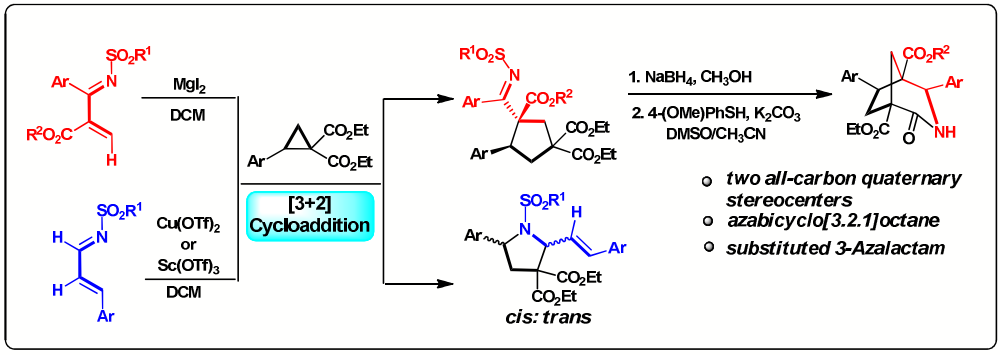
Nitrogen-containing carbocycles and heterocycles[1] are found in a variety of natural products and pharmaceutically relevant molecules.[2] For examples, gababutin analogues, constituting amine functionalized cyclopentanes, are having anti-inflammatory activity.[3] In addition, 1-sulfonyl pyrrolidine derivatives play a potential role for the treatment of neurological disorder.[4] Azabicyclic amino acid shows inhibitory activity against tumor cell.[5] For this interest, we have demonstrated Lewis acid catalyzed [3+2] cycloadditions reaction of DACs with 1-azadienes to synthesize a variety of imine functionalized cyclopentane and pyrrolidine derivatives *via* S_N2 and S_N1 fashion, respectively. Furthermore, two-step synthesis of valuable pharmaceutically relevant azabicyclo[3.2.1]octane, including two quaternary carbon stereogeniccenters has been achieved. In addition, we also report regioselective iodination of arenes of imine functionalized cyclopentane derivatives.



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P-99

Altered levels of C-reactive protein and leukocytes in COPD patients

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Introduction: Chronic obstructive pulmonary disease (COPD) is a collective term for emphysema, chronic bronchitis and some forms of bronchiectasis. It is characterized by chronic obstruction of airflow in lungs that interferes with normal breathing and is not fully reversible. Serum CRP (C-reactive protein) is a marker of inflammation.

Objective: The aim of the present study was to find whether there is a correlation between COPD and circulating levels of leukocytes. Also to characterize COPD patients on the basis of their CRP levels.
Methods: This study was done on 50 patients with clinical manifestations pointing COPD. 50 healthy individuals served as control. Blood sample was collected from each subject. Leukocytes were counted manually using hemocytometer and turk's stain. This was done on the same day of blood collection. Serum CRP level was studied by using ELISA technique. This study was done for both smokers and non-smokers.

Results: The leukocyte count and CRP levels were significantly higher in stable COPD in comparison to that of control group. Furthermore, their levels were significantly very higher in acute exacerbated COPD in comparison to that of both control group and stable COPD.

Conclusion: A significant association was found between raised leukocyte count in blood and severity of COPD; and raised CRP level and severity of COPD. Peripheral leukocyte count can serve as an indirect indicator of severity of COPD. Furthermore, this increase in CRP level was not related to smoking as the level of CRP was significantly raised both in smokers and non-smokers.

P-100

CHEMICAL SYNTHESIS OF CYSTINE MOTIFS

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We have made an attempt to develop simple and versatile procedure for synthesis of polypeptide cystine motifs. Conventional solid phase peptide synthesis methodology using Fmoc (9-Flurenylmethyloxycarbonyl) chemistry without side chain protection was employed in synthesis of these peptide motifs. We will be presenting characterization of the synthetic cystine motifs using chromatography and mass spectrometry. The present method has the following advantages over conventional method of synthesis of cystine peptide motifs: i) The method does not require oxidation procedure to facilitate foldings of polypeptide, ii) the method avoids disulfide isomerisation [1], thereby enhancing the overall yield of the desired peptides and iii) the method facilitates rapid synthesis of parallel polypeptides [2].

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P-101

Cp*Co(III) Catalyzed C—C Bond Formation of 1,3-Dicarbonyls To Terminal Alkynes: A highly Efficient way to Nakamura Reaction

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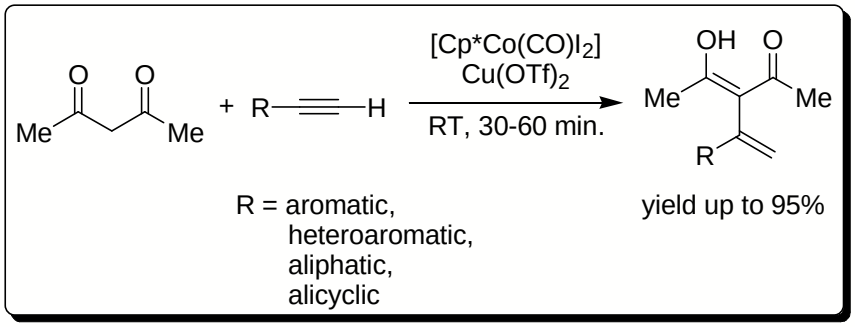
Abstract: In recent years, Co(III) catalyst [Cp*CoI_2(CO)], emerged as a robust, highly efficient and cheap catalyst for the construction of C—C bonds by direct/chelation-assisted functionalization of C—H bonds [1]. It was generally accepted fact that enolate anions do not undergo addition to un-activated alkynes and it has been a challenge to make the enolate anions reactive towards un-activated alkynes. Nakamura *et al*. successfully overcome this problem using In(III) salts at high temperature [2]. Encouraged by the seminal work of Nakamura, several groups reported this reaction in the presence of Re, Ir, Ru, Au etc [3]. To this end, we herein report for the first time a Co(III) catalyzed addition of acetylacetone with un-activated 1-alkynes at room temperature under solvent free condition, assisted by $Cu(OTf)_2$.



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P-102

Mycogenic silver nanoparticle from *Cladosporium* sp. FGCC/BLS 2: Process Optimization and antimicrobial applications

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Abstract: Mycogenic synthesis of metal nanoparticles finds diverse applications are non-toxic, safe and eco-friendly. In view of this, *Cladosporium* sp FGCC/BLS2 (Accession No. - KU752193.1) was isolated from soil, characterized and explored for the synthesis of silver nanoparticles (AgNPs) under optimized conditions. AgNPs synthesis was investigated using UV-visible spectroscopy, FTIR and TEM. Physico-cultural optimization exhibited rapid AgNPs synthesis within 8 hours under conditions of 2 mM $AgNO_3$, pH 11 and temperature 70^oC. FTIR spectra confirmed the presence of protein component bound to AgNPs which act as reducing and stabilizing agent. TEM analysis reported roughly spherical shape of AgNPs with average particle size ranges from 25 to 30 nm. Selected area electron diffraction pattern (SAED) revealed the crystalline nature of AgNPs synthesized using *Cladosporium sp*. AgNPs showed significant antibacterial properties against *Escherichia coli*, *Klebsiella pneumoniae* and *Staphylococcus aureus* as exhibite by disc diffusion, CFU counting and growth kinetics assay. Furthermore, AgNPs did not show any cytotoxic effects on human RBCs. Therefore, this novel fungal strain can be utilized for biofabrication of AgNPs under optimized conditions and have shown strong antibacterial action.

P-103

S-ACys: A NATURAL SHIELD AGAINST STRESS-INDUCED MYOTUBE ATROPHY

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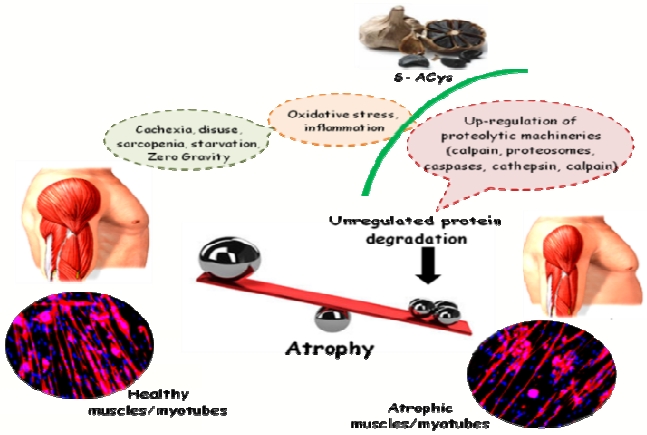

Abstract: Skeletal muscle atrophy/wasting/cachexia is a consequence of various physiological/pathophysiological conditions and is often associated with poor functional status and quality of life. In last two decades, new insights into the etiology of wasting have been reported, still it is an unresolved challenge. Review of 19 anti-atrophic drugs [1] and their mechanisms of action in regulating muscle mass makes it clear that atrophy is multifaceted problem and avaliable solutions are uni-directional. Increased reactive oxygen/nitrogen species and inflammatory molecules are key reasons in majority of clinical settings that induce muscle mass loss via up-regulating diverse protein catabolic machineries. S-ACys, a bioactive compound of Garlic (*Allium Sativum*), has a broad spectrum of properties but its role in muscle metabolism is unknown. In the present study we analysed the impact of S-ACys on H2O2- and TNF -induced cultured myotube atrophy. Various tools (immunocytochemistry, western blotting, bright field microscopy) have been used for confirming the onset of atrophic conditions in this study. Later, myotubes were pre-treated with S-ACys for 4h and then exposed with atrophic agents. Data suggest that H2O2-and TNF -exposure not only alter the myotubes morphology (reduced myotube length, diameter and fusion index) but also enhance the degradation of specific muscle proteins (myosin heavy chain and creatine kinase). Besides that markers of oxidative stress (lipid peroxidation, reduced glutathione and others), mitochondrial dysfunction (SDH) and injury (LDH) were observed imbalanced under such conditions. S-ACys pre-treatment of myotubes ameliorated the majority of derailed pathways induced by these oxidative and inflammation-mediated molecules. Our finding suggests that S-ACys has the tremendous potential to ameliorate the loss in myotube diameter and may prove beneficial in combating atrophy in different pathological conditions under oxidative/inflammatory stress-induced atrophy.

Key Words: S-ACys, skeletal muscle atrophy, oxidative stress, proteolysis

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P-104

Decarbethoxylative Arylation Employing Arynes: A Metal-free Pathway to Arylfluoroamides

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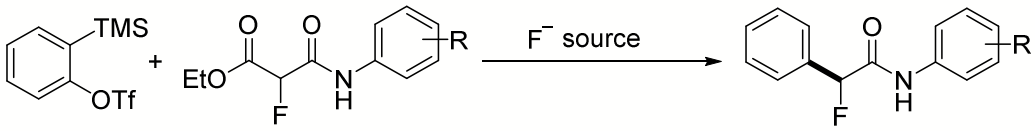
Arynes are highly reactive and valuable intermediate used in various fundamental organic transformations.[1] Owing to the pronounced electrophilicity of arynes and the highly strained triple bond in thering system, arynes have found widespread applications invarious bond-forming reactions, including pericyclic reactions,[2] insertion reactions,[3]multicomponent reactions (MCRs)[4] and arylation.[5] In C-arylation of 1,3-dicarbonyl species there is a potential competition between C-arylation and insertion which poses major limitation to this arylation strategy. This limitation is circumvented by selecting a suitable substrate which has secondary amide moiety,where exclusive arylation product was achieved. In this context, we established a facile transition metal-free decarbethoxylative arylation reaction for the synthesis of α-aryl-α-fluoroamides from fluoromalonamates under ambient reaction conditions using aryne as an electrophilic arylating agent.[6] This decarbethoxylative arylation process proceeds under mild conditions and provides a practical and effective entry to a wide range of α-aryl-α-fluoroacetamides.



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P-105

Rapid and selective synthesis of spiropyrazolines and pyrazolylphthalides employing Seyferth–Gilbert reagent

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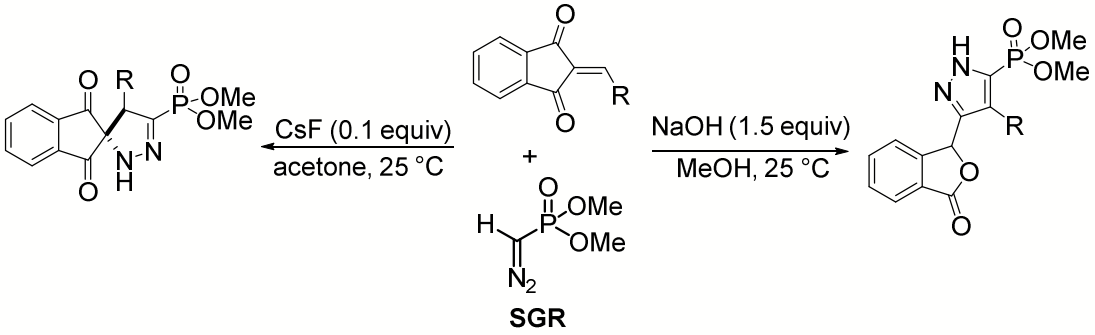
Dimethyl(diazomethyl)phosphonate (Seyferth–Gilbert reagent, SGR) have been extensively employed for the convenient generation of homologated terminal and internal alkynes from aldehydes and ketones under ambient reaction conditions.[1,2] Subsequently, the 1,3-dipolar cycloaddition reaction involving diazomethylphosphonate (DAMP) anion, the key intermediate generated from these reagents, and various activated olefins has emerged as an important methodology for the synthesis of phosphonylated pyrazoles.[3]Although great progress has been achieved in the synthesis of phosphonylpyrazoles using Seyferth–Gilbert reagent, relatively a few protocols are reported for the synthesis of spiropyrazolines. We disclose a highly effective and mild protocol for the synthesis of phosphonylspiropyrazoline derivatives 2-arylideneindane-1,3-dione with dimethyl diazomethylphosphonate and quite interestingly, further investigations revealed an attractive product selectivity switch on changing the reaction conditions, introducing a new and efficient route to pyrazolylphthalides.[5]The reaction of 2-arylideneindane-1,3-dione conducted with dimethyl diazomethylphosphonate in acetone gave spiropyrazolineindane-1,3-dione, while the use of basic methanol provided hitherto unknown pyrazolylphthalide derivatives.



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P-106

Transformation of glycals to chiral fused aromatic cores via annulative pi-extension reaction with arynes

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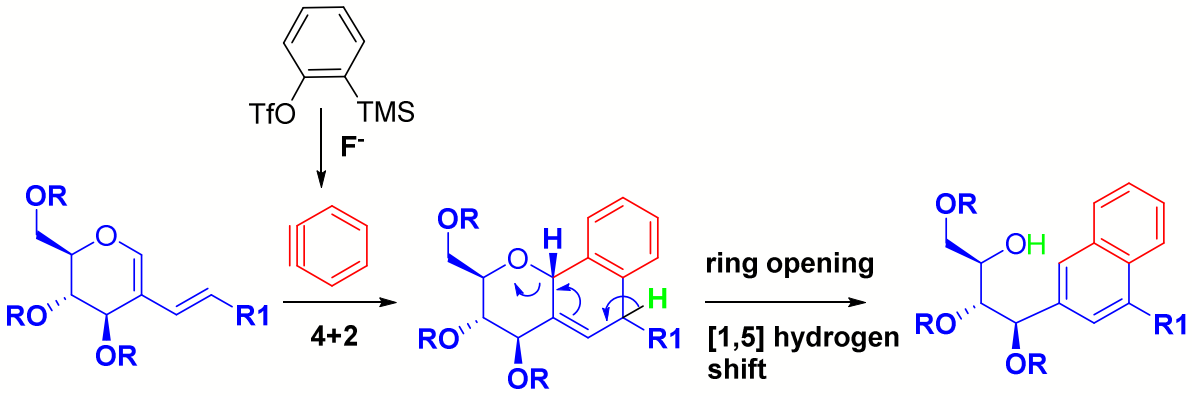
Carbohydrate derived chiral intermediates which contain arrays of defined stereocenters have found enormous applications in organic synthesis due to their inherent functional group, stereochemical and structural diversities as well as their ready availability.[1]Stereodiversity of these classes of molecules have motivated synthetic organic chemistry over the years.[2] One major challenge is control of relative configuration during construction of acyclic fragments.[3] Here we show that benzynes can be captured by glucal based diene to form oxadecaline core and subsequently annulative pi-extension can take place opening up the sugar ring in stereospecific fashion. Additionally, we embarked on this study to: (i) gain new insights about benzynechemoselectivity and (ii) synthesis of fused aromatic moiety flanked by two achiral side chains with tunable defined stereochemistry



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P-107

Three-Component Domino Approach for the Synthesis of Disubstituted Pyrazoles by using diazosulfone as Diazomethane Surrogate

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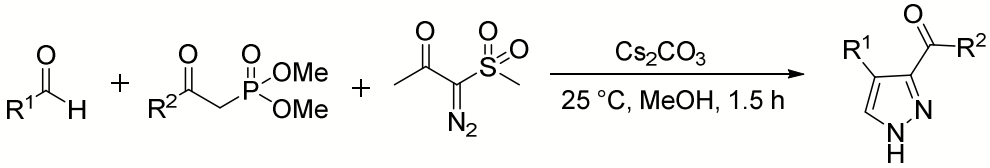
The simplest 1,3-dipolar reagent discoverd was diazomethane which was used for [3 + 2] dipolar cycloadditions with alkenes and conjugated enynesulphone to access pyrazolines and pyrazoles, respectively.[1,2]One of the major disadvantages of using diazomethane is thepreparation of potentially explosive solutions of diazomethane.[3]Although α-diazo-β-ketosulfones have been explored in intramolecular cyclopropanation, carbene insertion reactions, relatively very limited methods have been reported for 1,3-dipolar cycloaddition reactions.[4] In the context of our interest in the chemistry of diazocompounds, we turned our attention towards the development of novel cycloaddition reactions involving diazosulfones. Interestingly, our efforts culminated in the development of an efficient three-component domino reaction for the synthesis of 3-acyl, 4-aryl pyrazoles under mild conditions.[5]The process involves the HWE olefination/1,3-dipolar cycloaddition/desulfonation cascade that utilizes β-ketopropyldiazomethylsulfone as a synthon for the diazomethane in methanol. These results broaden the emerging role of the β-ketopropyldiazomethylsulfone as a diazomethane surrogate in domino fashion.The reaction is practicallydomino one-pot process, does not require a catalyst or the isolation of the potentially toxic and explosive gaseous intermediate diazomethane, and proceeds under basic condition in open flask. Attractive features of this process are its versatility, the readily available starting material and the efficiency to create a complex core in a single operation.



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P-108

Atom economical and stereoselective synthesis of Spiropyrrolidinochromanones based on Ugi four component reactionfollowed by phosphine catalysedintramolecular cyclization

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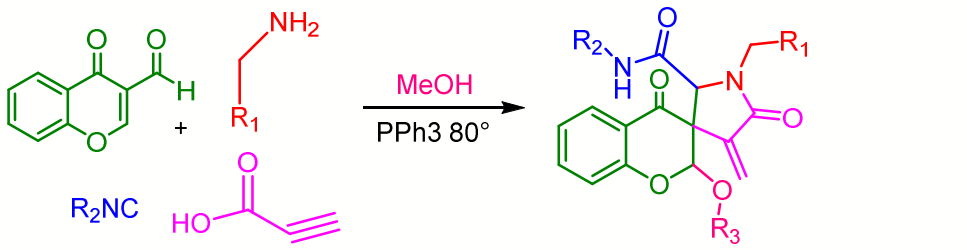
Abstract: Spiroheterocyclic structures are common scaffolds being used in drug discovery of their three- dimensionalitySpiroheterocyclic Structures areCommon Scaffold of many bioactive natural product.

this report describes novel, efficient stereoselective, one – pot, two step, sequential synthesis of biologically relevant spiropyrrolidinochromanones. This protocol involves the Ugi four-component reaction (U-4CR) phosphine catalysed highly stereoselectivefollowed by nucleophilicconjugated addition andintramolecular cyclization. In addition, it is interesting to report that solvent plays the role of nucleophile, thus providing a highly atom – economical and environmentally benign approach towards the synthesis of spiropyrrolidinochromanones.



R1,=benzyal amine
R2,=tert butyl,cyclohexyal,isocynide

R3,=methanol,ethanol,isopropanol

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P-109

Synthesis of 4-fumarate substituted acyl coumarins by a cascade reaction of acyl coumarin with Alkyne Derivatives

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Abstract: Coumarin derivatives have proven to be useful motifs and exhibit a wide range of biological/ pharmacological activities, like antioxidant, anti-HIV, anti-Alzheimer, anti-inflammatory, antibacterial, and antiviral activities.Coumarin derivatives also have attracted attention due to interestingphotophysical, photochemical and photobiological properties of 7-(diethylamino)/ 7-hydroxy coumarin and their derivatives. Coumarin derivatives with substitution both in aromatic and heterocyclic ring have been prepared due to their variety of application. A number of 4- substituted coumarin derivatives have been reportedas tubulin-targeting antitumor agents.

Organocatalytic triphenylphosphinecatalyzed cascade reactions of acylcoumarins with electron deficient alkynes like dialkyl acetylenedicarboxylates has been achieved to give the 4-fumaratesubstituted acyl coumarins in moderate to high yields. The reactions were attempted under a variety of conditions by changing molar ratio of substrates, solvents and also the reaction temperature to identify appropriate reaction condition to achieve the desired synthesis.All the products have been characterisedspectroscopically using PMR, CMR, IR and HRMS. X-ray analysis of one of the products has also confirmed the structure. Mild reaction conditions, good atom economy and easy handling as well as a wide substrate scope are some of the salient features of the methodology. Details will be presented.

P-110

Lead optimization of 4-aminoquinoline based molecular hybridsaspotentantimalarial agents.

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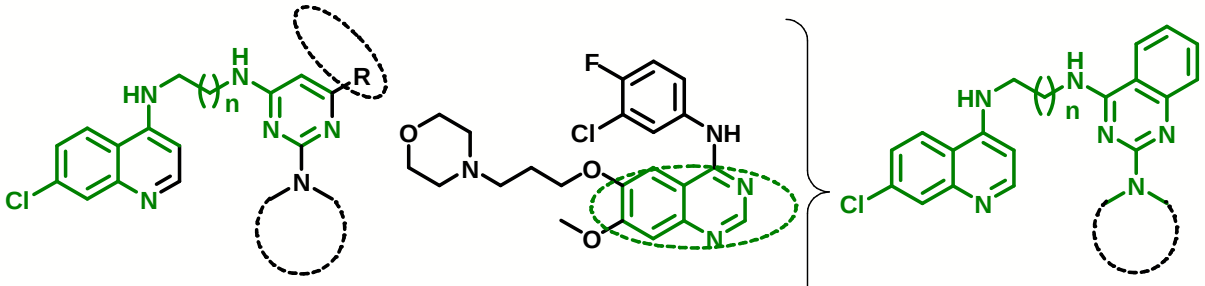
According to WHOworld malaria report, there were 429,000 deaths and 212 million new cases of malaria were reported in 2015. Economically deprived nations were the most effected.[1]Chloroquine, a 4-aminoquinolines based molecule, have been used as a cheap drug for a long period, but resistance developed by *P. falciparum* against this drug leads to search for alternative molecules.[2] Mechanistic studies shows thatchloroquine (CQ) prevents the hemozoinformation by binding with heme inside the digestivefood vacuole (DV) of the parasite. This leads to the accumulation ofheme in the DV, which is lethal to the parasite. In the CQ resistant *P. falciparum*, mutated *Pf*-CRT is the one of the main cause of resistance, which efflux CQ from DV and prevents the accumulation of CQ inside DV.[3]Research shows that use of *Pf*-CRT inhibitorin combination with CQ can solve the CQ resistance.Gefitinib, a quinazoline based anticancer drugcan reverse the CQ resistance in the parasite.[4] Moreover,our group reported the AQ-pyrimidine hybrids as excellent antimalarial agents against both CQ resistant and sensitive strain of *P. falciparum.*[5] and based on QSAR study; incorporation of hydrophobic moiety on the 4th position of pyrimidine can improve antimalarial activity.[6]By these facts we hypothesised that, the AQ-QN hybrids can show improved antimalarial activity. Here we report the design andsynthesis of AQ-QN hybrids with potent antimalarial activity against both sensitive and resistance strains of *Plasmodium*.



ACS Med. Chem. lett., 2012
IC_{50}: 6-440 (D6) nM
IC_{50}: 16-1240 (W2) nM

Gefitinib

AQ-QN Hybrids
IC_{50}: 11.6 -169 (D6) nM
IC_{50}: 7.5-1600 (W2) nM
IC_{50}: 0.58-100 (NF54) nM

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P-111

Green Chemistry approach: novel synthesis and larvicidal activity of anthracene-9,10-dione marine basednatural products and their analogues

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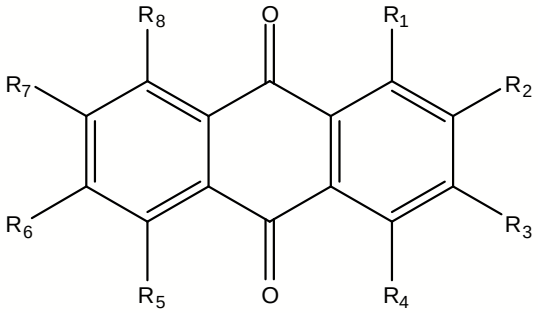
Anthraquinones are the largest group of natural pigments of quinoid nature [1].9,10-Antraquinones are a class of secondary metabolites that have been found in plants and marine sources[2].A number of biologically active compounds with varying degrees of action, such as anti-tumor, anti-cancer, anti-microtubule, anti-proliferative, cytotoxic, photo protective, as well as antibiotic and antifouling properties, have been isolated to date from marine sources[3].These compounds are characterized by a core structure of anthracene-9,10-dione and are diversified by many library of products.Synthesis of anthroquinone from pthalicanhydride react with substituted phenol via green chemistry approach without solvent. Their structures were characterized by FTIR, ^{1}H NMR, ^{13}C NMR, and HRMS.The diversity of the anthraquinoid compounds relies on the nature and the position of the substituents, replacing the H atoms on the basic structure (R1 to R8), as diverse as: –OH, $–CH_3$, $–OCH_3$, $–CH_2OH$, –CHO, –COOH, or more complex groups [4-6]. In order to discover the new larvicidalactive molecules from our library of our anthracene-9,10-dione and some of compound exhibited above 90% of mosquito larvicidal activity.



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P-112

Electron Transfer Dissociation Mass Spectral Cleavage of Lanthionine Bridges of Synthetic and Natural and Synthetic (Lanti) Peptides

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(Corresponding author's Email.id: hanumae@gmail.com)

In the present study we have investigated ETD (Eelctron Transfer Dissociation) mass spectrometric method for structural analysis of Lanthionine containing peptide. Synthetic Lanthionine containing peptide was obtained by alkali induced Lanthionine formation from corresponding disulfide peptide, natural Lanthionine containing peptide was obtained from chemical cleavage of Nisin, a well known Lantibiotic. Combination of ETD and CID method was performed to prove the radical initiated cleavage under mass spectrometric condition. The cleavage preferentially gives an even electron containing 'z' ions with Dha (dehydroalanine) and odd electron containing 'c' ions with Cysteine thiol radical upon cleavage of Lanthionine.

CID (Collision Induced Dissociation) of second generation product ions further provides confirmation of formation of Dha (dehyderoalanine) and Cysteine thiol radical from Lanthionine. In the case of an intramolecular Lanthionine containing peptides radical cascade reactions leads to formation of an odd electron 'z' ion with Cysteine thiol radical.

The present report highlights the advantages of ETD-MS in characterization of Lanthionine peptides and may assist rapid characterization Lantipeptidomes of bacteria.

P-113

Isolation and NMR Studies of Aliose- A Novel Hexasaccharide from Donkey's Milk

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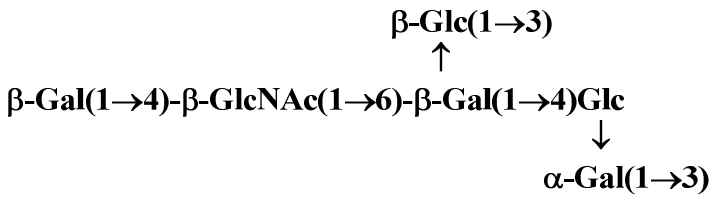
Abstract: One of the most striking features of milk is the diversity and abundance of complex glycans that include free milk oligosaccharides, glycoproteins, glycopeptides and glycolipids. Milk oligosaccharides are indigestible to the infant and play multiple roles in the health of the neonate by stimulating growth of selected beneficial bacteria in the gut, participating in development of the brain, enhancing intestinal epithelial barrier function, exerting potent biological activities such as anti-tumor, immunological, anti-complimentary, anti-cancer, anti-inflammatory, anti-coagulant, hypoglycemic and antipathogenic activities. Donkey milk oligosaccharideshave ability to stimulate specific and non-specific immunological resistance and prevention of athereosclerosis. Keeping above mentioned biological activities of donkey's milk oligosaccharides in mind we have isolated a novel hexasaccharide namely **Aliose** from Donkey's. The structure of Aliose was established by comparing the chemical shift data of ring protons and anomeric signals in the ^{1}H NMR of Aliose and Aliose acetate which was supported by ^{13}C NMR, 2D NMR (COSY, TOCSY and HSQC) and Mass spectrometry. Splitting pattern of anomeric signals in ^{1}H NMR confirmed the configuration of glycosidic linkages. The structure deduced by the NMR experiments was also confirmed by the FAB-MS of Aliose which contains M^{+} and other Mass ion fragments confirming the deduced structure. In lights of result obtained from above physico-chemical techniques, chemical degradation and chemical transformation the structure of Aliose was deduced as-



Keywords: Donkey milk, Oligosaccharides, Aliose.

P-114

Isolation Of Novel Milk Oligosaccharide From Mare Milk

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Carbohydrate-containing moieties exist in the form of glycosides, glycoprotein glycoconjugates, oligosaccharide etc. In all these moieties the glycan portion is present as oligosaccharide. Free oligosaccharides are natural constituents of all placental mammals' milk and also found in bacteria, fungi, plant, etc. Milk oligosaccharides have establish themselves as an effective class of organic bimolecular impacting various physiological and pathological processes such as bimolecular recognition,signal transaction, differentiation and developmental events and exhibit various biological activities such as antitumor, immune-stimulant, anti-cancer, anti-complimentary, anticoagulant, anti-inflammatory, hypoglycemic, antiviral and immunological activities.Mare milk oligosaccharides is plentiful of fat resembling substances that contributein transfer of certain nerve impulses and the regulation of blood pressure. Mare milk is also used as antioxidant,lipid lowering agent and mineral absorption regulating agent. With a view to isolate biologically active novel oligosaccharide**(Labiose)** mare milk was collected and processed by the Kobata and Ginsburg method and followed by gel filtration, HPLC and column chromatography. The HSQC spectrum of acetylated labiose showed the presence of eight cross peaks of anomeric protons and carbons in the respective region at δ5.38 x 90.3, δ4.65 x δ95.4, δ4.53 x 102.1, δ 4.73 x 102, δ 4.70 x 102, δ5.387 x 90.30, δ 4.65 x 95.5 and δ 5.25 x 92.1 suggesting the presence of eight anomeric protons and carbons in it. The results obtained from chemical transformation, chemical degradation along with spectroscopic data suggested that it was a heptasaccharide in its reducing form. The glycosidic linkages were confirmed by the splitting pattern of anomeric signals. Further the structure was confirmed by the 2D NMR studies involving COSY, TOCSY, HSQC techniques along with mass spectrometry. The structure of **Labiose** was confirmed as under;

$$\alpha Gal(1\rightarrow4)$$
$$\uparrow$$
$$\alpha Gal(1\rightarrow4)\beta Glc(1\rightarrow6)\beta Gal(1\rightarrow3)\beta GlcNAc(1\rightarrow6)\beta Gal(1\rightarrow4)Glc$$

Key Words : Mare milk, oligosachharide, labiose.

P-115

^{13}C NMR Studies of Pregnanes

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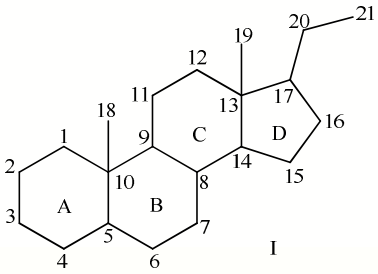
Pregnanes are C-21 steroidal compounds having the usual perhydro-1,2-cyclopentano phenanthrene ring system with β-oriented angular methyl groups at C-10 and C-13 and a two-carbon side chain at C-17. Pregnanes and their glycosides are widely distributed in the plant kingdom and in some marine organisms, and are known to possess interesting biological activities like anti-tumour, anti-cancer, and anti-proliferative activities. Certain plant families like Asclepiadaceae and Apocynaceae, have been found to be rich sources of these compounds. The biological activities of pregnanes have generated great interest of the chemists for solving the structural diversities of these pregnanes and their glycosides.Modern NMR instruments, equipped with high field resolution and FT technology, and mass spectrometry, have greatly revolutionized and enhanced the speed of identification of these compounds. Although ^{13}C NMR and ^{1}H NMR spectroscopy are complementary to each other, but without the interpretation of ^{13}C NMR data it is not possible to elucidate the complete structure of pregnanes because it provides the complete information regarding tertiary and quaternary carbons, which is a limitation for ^{1}H NMR. More over the range of chemical shift dispersion of ^{13}C NMR is δ0 – 200, which is limited to δ0 – 10 in ^{1}H NMR, which resolves the problem of overcrowding of signals in a particular chemical shift area.The ^{13}C chemical shifts of various compounds have been used over years to create computer-readable spectroscopic databases. The structure elucidation through automated analysis of the spectroscopic data is a technique with considerable potential. For this purpose, we have collected the ^{13}C NMR data of pregnanes reported over the last 30 years, along with their structures in a tabulated form, so that it may be used to develop a computer-generated program for the identification of pregnanes.



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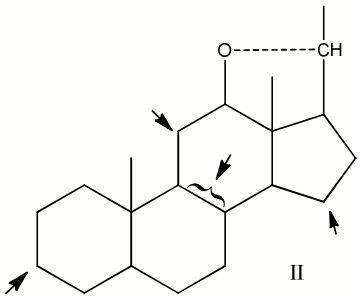

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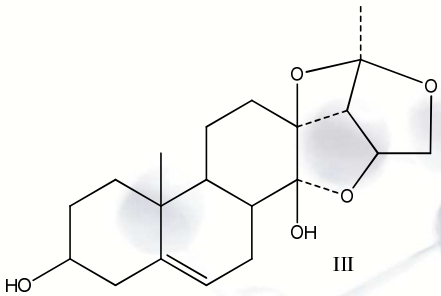

III

Figure I, II, III – Basic Skeletons of Pregnanes

Keywords: ^{13}C NMR, Pregnanes, Spectroscopic-databases.

P-116

ISOLATION AND STRUCTURE ELUCIDATION OF NOVEL GOAT MILK OLIGOSACCHARIDE BY NMR

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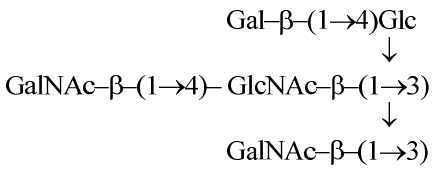
Milk oligosaccharides have been known to have many biological functions including as prebiotics, as receptor analogs to inhibit the binding of pathogens and as components involved in modulating the immune system. Goat milk is rich source of oligosaccharide which reduces intestinal inflammation as well as shows anticarcinogenic, antioxidant, antibacterial, antimicrobial and antiviral activity. In present study, we have isolated a novel milk oligosaccharide namely Boviose from goat milk. For this purpose goat milk was collected and processed by modified method of Kobata and Ginsburg followed by gel filtrate chromatography, acetylation and column chromatography of derivatized oligosaccharides and subsequent HPLC. Structure elucidation of the isolated oligosaccharide was based on the result obtained from spectroscopic techniques like ^{1}H and ^{13}C, 2D-NMR (COSY, TOCSY, HSQC and HMBC) and ES-MS along with chemical degradation and chemical transformation. The ^{1}H and ^{13}C NMR spectra of compound showed six anomeric proton and carbon peaks at δ6.23(1H), δ5.65(2H), δ4.61(1H), δ4.58(2H) and δ88.93(1C), δ91.35(2C), δ101.63(1C), δ101.77(2C) respectively confirming the presence of five monosaccharide in Boviose thus confirming the structure of Boviose as pentasaccharide in its reducing form. The splitting pattern of anomeric proton signals confirmed the configuration of glycosidic linkages. All the signals of ^{1}H- and ^{13}C-NMR and position of glycosidic linkages were assigned by COSY, TOCSY, HSQC and HMBC spectra. In the light of foregoing evidence the structure of the isolated pentasaccharide was deduced as:



Boviose

Key words: Prebiotics, inflammation, Boviose, Goat milk and Kobata and Ginsburg

P-117

Copper-Promoted Regioselective Intermolecular Diamination of Ynamides: Synthesis of Imidazo[1,2‑a]pyridines

Vikas Dwivedi, Ravi Kumar, Kavita Sharma, Balasubramanian Sridhar, and Maddi Sridhar Reddy*

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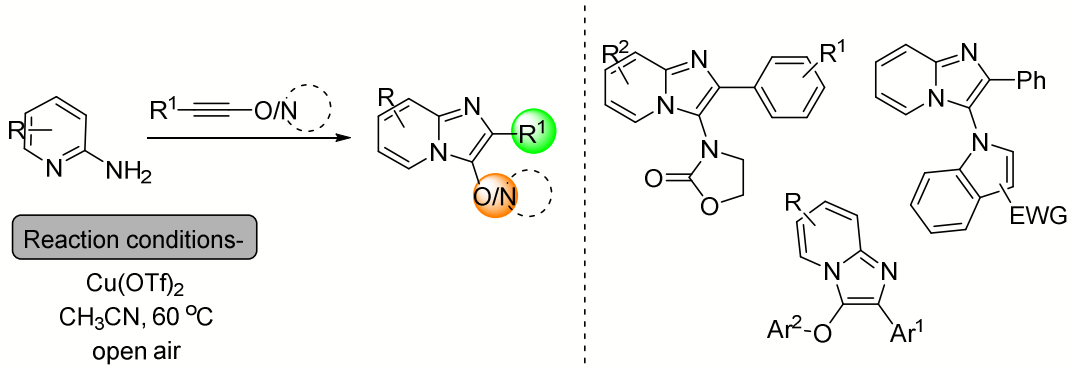
The imidazo[1,2-a]pyridine[1]skeleton is a class of nitrogen comprising heterocycles which is composed of pyridine and imidazole rings, displaying numerous biological activities[2],such as antitumor, antiparasitic, antimicrobial, fungicidal, anti-inflammatory and hypnotic, consequently present in several marketed drugs[3]such asalpidem, zolpidem, necopidem, saripidem, zolimidine, and olprinone. Here we have presented a facile access to 3-heterosubstituted (3-oxazolidinonyl/indolyl/phenoxy) imidazo[1,2-a]pyridines from readily available 2-aminopyridines and electron-rich (internally activated) alkynes like ynamides/ynamines/ynol ethers via $Cu(OTf)_2$-mediated intermolecular diamination under aerobic conditions. The reaction is highly regioselective, owing to internal electron bias, and thus led to a single regioisomer with heterosubstitution at C3.



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P-118

An efficient metal-free C-arylation ofketoamides employing diaryliodonium salts

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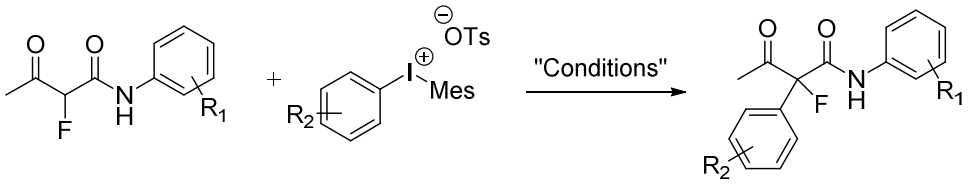
Hypervalent iodine(III) compounds have recently been demonstrated as efficient reagents for a wide range ofcarbon-carbon bond formation in synthetic organic chemistry.[1]Iodine(III) reagents with two carbon ligands have properties resemble to those of Hg, Pband Pd complexes, and can be employed in reaction pathways that are similar to metal-catalyzed reactions.[2]. Recent advances in C-arylation methodology with carbon nucleophiles have mainly relied on the use of transition metal catalysis. However, novel transition metal-free reactions have a potential environmental and economic benefit as they avoid precious metal catalyst systems and metal-remediation steps in synthesis. Symmetric diaryliodonium salts are well-known to participate in C-arylation reactions under relatively mild conditions, and this underpins a general strategy to metal-free arylation of diverse nucleophiles.[3] On the basis of literature survey and recent success in the arylation of alkoxide nucleophiles with unsymmetrical aryl-(mesityl)iodonium salt electrophiles, we turned our attention to C- nucleophiles, and selected α-fluoro-β-ketomides as a model substrate for our studies.Interestingly,an attractive metal-free coupling of α-fluoro-β-ketomides with unsymmetric aryl(auxiliary)iodonium salts has been developed in our laboratory.[4]



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P-119

β-CD/CuI catalyzed regioselective synthesis of iodo substituted 1,2,3-triazoles, imidazo[1,2-a-pyridines and benzoimidazo[2,1-b]thiazoles in water and their functionalization.

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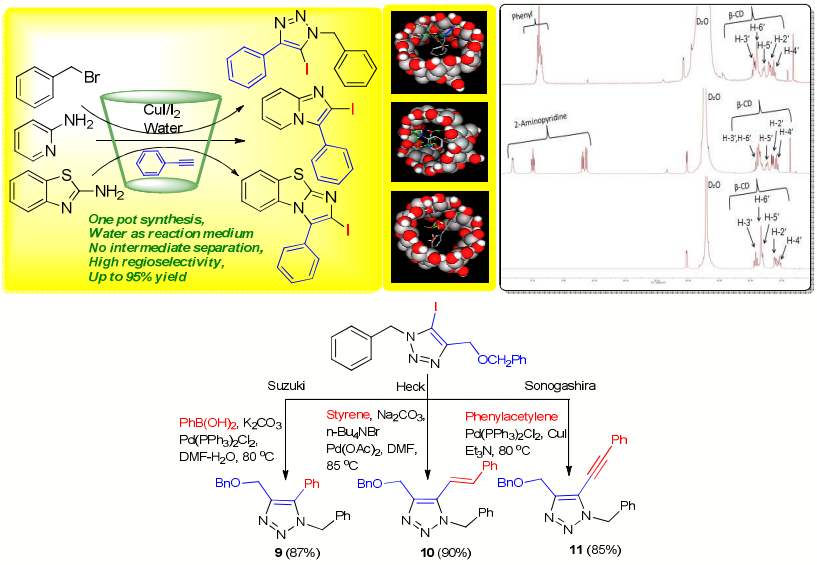
An environment benign process has been developed for the regioselective synthesis of 5-iodo-1,4-disubstituted-1,2,3-triazoles catalyzed by CuI/β-CD in water. Moreover, the process was manifested for the efficient synthesis of 2-iodo-imidazo[1,2-*a*]pyridines and 2-iodo-benzoimidazo[2,1-*b*]thiazoles in aqueous medium. Additionally, the iodinated derivatives were successfully modified *via* palladium catalyzed coupling reactions like Suzuki, Heck and Sonogashira. The salient features of this methodology are *in-situ* formation of 1-iodoalkyne & alkyl/aryl azide under mild reaction conditions, high regio-selectivity and use of water as a greener solvent.



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P-120

Isolation & Structure Elucidation Of Novel Hexasaccharide From Cow Colostrum

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Colostrum is the first natural food for the newborn infants. Colostrum is a source of proteins, carbohydrates, fat, vitamins and minerals and also contains several biologically active molecules. The bovine colostrum oligosaccharides are used in treatment of inflammatory bowel disease and human gastrointestinal health. It also prevent adhesion of pathogenic microbes and maintaining good health in breastfed infants. Moreover the biological importance of cow milk given in ayurveda is enormous. So we have isolated a novel hexasaccharide namely **Tososе** from cow colostrum. For this purpose cow colostrum was processed by modified method of Kobata and Ginsburg followed by gel filtration, column chromatography and its subsequent HPLC. The HSQC spectrum of acetylated Tososе showed the presence of six cross peaks of seven anomeric protons and carbons in their respective region at δ6.15x89.88, δ5.67x90.35, δ5.36x89.12, δ5.35x89.12, δ4.58x101.23 and δ4.50x100.83 suggested the presence of seven anomeric protons and carbon in Compound Tososе in its reducing form. The presence of six doublets for seven anomeric protons at δ6.15(1H), δ5.67(1H), δ5.36(1H), δ5.35(1H), δ4.58(1H) and δ4.50(2H) in the ^{1}HNMR of Tososе Acetate in $CDCl_3$ at 300MHz.confirmed that it was a hexasaccharide. The configuration of glycosidic linkages was confirmed on the basis of splitting pattern of anomeric signal in ^{1}H NMR spectrum. The sequence of sugar was confirmed by mass fragments generated by FAB-MS and chemical degradation. On the basis of the result obtained from the above experiments, structure of novel oligosaccharide Tososе was established as:

Gal-β-(1→2)-Gal-α-(1→4)-Glc-α-(1→3)-GalNAc-β-(1→3)-GalNAc-β-(1→4)-Glc

TOSOSE

Key word: colostrum, hexasaccharide, ^{1}H NMR

P-121

Isolation, Purification and Structure elucidation of novel Donkey milk oligosaccharides

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A large number of oligosaccharides have been isolated from milk of different ruminants and they have shown unique biological activities such as anti-tumor, anti-cancer, anti-inflammatory, and, antioxidant. Donkey's milk oligosaccharides have ability to stimulate non-specific and specific immunological resistance and proposed to be very helpful in cure of AIDS patients and in prevention of atherosclerosis. Simultaneously it also contains sialytated and fucosylated oligosaccharide, which are useful for cosmetic purpose. So, donkey's milk processed by Kobata and Ginsburg method followed by various column chromatographic techniques resulted in the isolation of a novel milk oligosaccharide, **VULGOSE**. The presence of five anomeric signals in ^{1}H NMR at δ5.25, δ4.70, δ4.55, δ4.49, and δ4.48 and three signals for five anomeric carbons in ^{13}C NMR at δ102.9, δ95.8 and δ91.8 of vulgose acetate confirmed that it was a tetrasaccharide. Comparison of ^{1}H NMR signals of vulgose and vulgose acetate supported by 2D NMR data in COSY, TOCSY, and HSQC experiments and structure reporter groups. The splitting pattern of anomeric signals in ^{1}H NMR confirmed the glycosidic linkages in vulgose. The tetrasaccharide nature of vulgose was also confirmed by mass spectral data having [M+K] and [M+H]. Moreover, it was the first compound reported from any milk in which the reducing end of any milk oligosaccharides contain GalNAc-(1→4)-Glc instead of Gal(1→4)Glc. The structure of isolated novel oligosaccharide (VULGOSE) was interpreted as under:

GalNAc--β-(1→4)-Glc-β-(1→3)-GalNAc-β-(1→4)Glc

VULGOSE

Key words- Milk Oligosaccharides, 2D NMR and Vulgose

P-122

Unprecedented concomitant formation of Cu_2O-cyclodextrin nano superstructures during the aerobic oxidation of alcohols and their catalytic use in propargylamination reaction: A simultaneous catalysis and metal waste valorisation (SCMWV) method.

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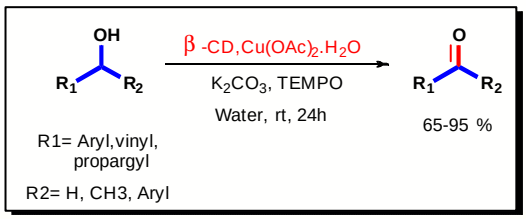
Aerobic oxidations of alcoholan important organic transformation both in Industry and Accademia[1].Traditionally, methods based on the use of chromium and manganese oxides, Fetizon's reagent, hypervalent iodine reagents (IBX, Dess – Martin reagent) and Swern oxidation reagent are known for aerobic oxidation reactions[2]. However, these methods use toxic solvents and generate copious amounts of hazardous metal waste, which prevents them from being adopted for large scale syntheses. Besides, these reactions are also often carried out with high concentrations of bases and environmentally unfriendly organic solvents. Unfortunately, despite the substantial benefits, several factors such as fire (or) explosion hazards of organic solvents, the need for modified plant designs along with specialized equipment limit its large-scale utility. Additionally, requisites such as elevated temperatures and pressures (to compensate the Limiting Oxygen Concentrations) for achieving significant conversions escalate the overall cost of the process. Thus, on account of these drawbacks, aerobic oxidations are seldom preferred in the pharmaceutical and fine chemical industry. Our interest is to develop the copper-catalyzed oxidation systems with economically and environmentally benign oxidants such as oxygen, whose reduction product is water. Therefore, considering theadvantageous characteristics of copper-CD and the limitations of aerobic oxidations, we develop copper- β-cyclodextrin combination for biomimetic oxidation of alcohols in presence of K_2CO_3 as base under aqueous conditions at room temperature. During such an effort, we serendipitously discovered the unusual concomitant formation of Cu_2O-CD nanosuperstructures while carrying out the aerobic oxidation of alcohols in water using Copper-CD complex.



Scheme 1. Aerobic oxidation of alcohol using copper-CD complex.

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P-123

COUMARIN–TRIAZOLECONJUGATES AS ANTIFUNGAL AGENTS

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Click chemistry has risen as a quick and capable way to deal with the synthesis of novel compounds with desired properties. The idea of "click chemistry" was authored in 2001 by Sharpless and coworkers[1] to depict an arrangement of “near perfect” bond-forming reactions which were exceptionally specific, high yielding, and wide in scope and describes chemistry custom fitted to create substances rapidly and dependably by consolidating little units.

In the course of recent years, 1,2,3-triazoles shows wide scope of biological applications including anti-tubercular, anti-bacterial, anti-allergic, anti-HIV, anti-fungal activity and α-glycosidase inhibitor activity[2]A library of coumarin derivatives with 1,2,3-triazole moiety were synthesized and proved to possess antifungal activity.[3] Therefore the incorporation of triazole moiety is essential for the enhancement of activity. Herein, we would like to report synthesis and bio-evaluation of novel 1,2,3-triazoleincorporated coumarin derivatives*via* click chemistry approach and will be presented.

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P-124

A supramolecule based ruthenium catalyst for selective aerobic oxidation of alcohol in aqueous medium: Further tuned for one pot oxidation and reduction reaction using same catalyst.

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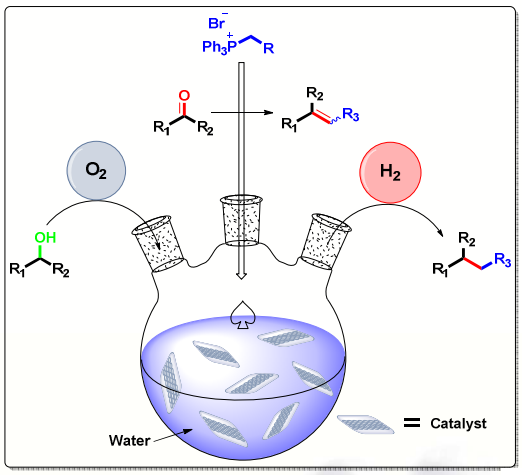
Abstract:Sustainable organic synthesis plays vital role in the improvement and sustainability of the modern society. In this context, the development of sustainable oxidations transformations, in particular, the oxidation of alcoholsis of high demand asit provides access to the building blocks for the synthesis of various natural, unnatural and biologically active molecules.Moreover, aerobic oxidation of alcohols has been more focused in the recent years, since the use of inexpensive and abundant molecular oxygen as terminal oxidant and water as by product of the oxidation reaction. However, to carry out large scale aerobic oxidations in flammable solvents, *Limiting Oxygen Concentrations* are to be maintained to prevent combustion reactions. Additionally, controlling the over oxidation of aldehydes into acid and the selective oxidation of alcohols in the presence of oxidisable functional groups are challenges that need to be addressed. Considering the drawbacks of existing methods, wedevelopeda novel efficient catalyst for selective aerobic oxidation alcohols under ambient conditions using water as benign solvent.The developed catalyst was found to be promising in catalysing both oxidation and reduction reactions under one-pot conditions.This unique ability of the catalyst to switch between oxidation and reduction reactions simply by changing O_2 and H_2 atmospheres with a balloon assembly exemplifies its versatility. Moreover catalyst was found to be easily recovered and recyclable up to five cycles.



Scheme: General reaction scheme.

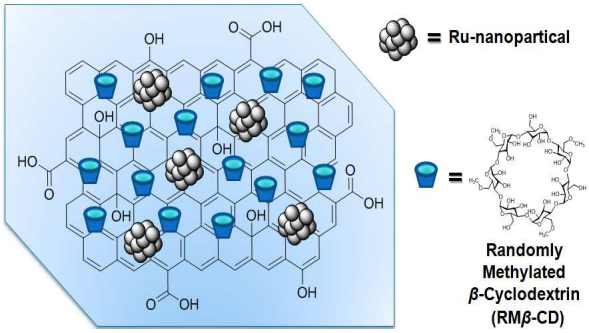


Figure: Graphical rGO@Ru-RMβ-CD catalyst representation

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P-125

Efficient atom and step economic (EASE) synthesis of the "smart narcoleptic drug"Modafinil

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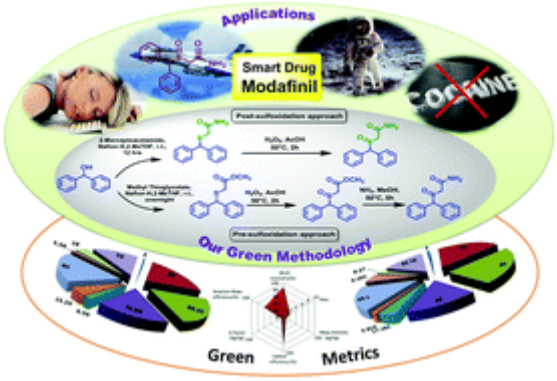
Abstract: Modafinil(2-[(diphenylmethyl)sulfinyl]acetamide, MOD) is a key psychostimulant drug used for the treatment of narcolepsy and other sleep disorders that has a very low addiction liability.[1] Recently, MOD has been clinically investigated for the treatment of cocaine addiction and used by astronauts in long-term space missions. In order to increase reaction efficiency over traditional previous syntheses and in continuation of our previous efforts to synthesize biologically andmedicinally important compounds, we have developed a synthetic strategy for "smart drug"Modafinil.[2] An efficient atom and step economic (EASE) synthesis has been carried out by the direct reaction of benzhydrol and Nafion-H along with post-sulfoxidation. This protocol exhibits improved sustainability credentials. We have also developed a superior pre-sulfoxidation approach for the synthesis of Modafinil.[3]



≠ Presenting author, DOB: 17-11-1992.

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P-126

Pyranone derived Donor-Acceptor Based Fluorescent Dyes for Live cell Imaging Applications

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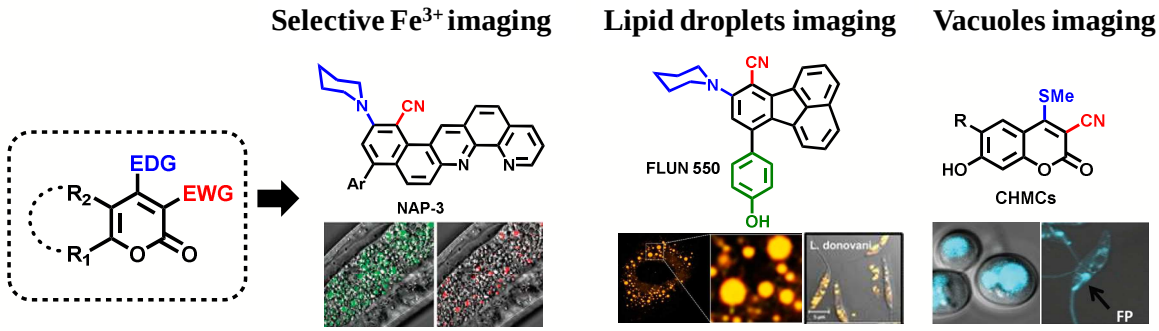
Fluorescence imaging techniques have emerged as an inevitable tool for visualising and analysing the live cells.[1] Fluorescent molecules possess high sensitivity, specificity, fast response and technical simplicity, thus, are used as fluorescent probes for imaging of cell organelles with the changes in microenvironment as well as sensing of metal ions in cells.[2] Our research group is involved in the design and synthesis of small molecule fluorescent probes derived from donor-acceptor π-conjugated pyranones for their bio-imaging, chemo-sensing and material applications.[3-8] We have developed a new class of fluorescent molecules e.g. FLUN-550 for imaging of lipid droplets, NAP-3(the first dual colorimetric and ratiometric fluorescent probe) for detecting the iron (III) and CHMCs for vacuoles imaging. Thus, our research is focused on synthesis and design of fluorescent probes and their application in biological systems. These details will be highlighted in the poster presentation.



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P-127

HIGHLY EFFICIENT TANDEM SYNTHESIS OF TRIAZOLE-PYRAZOLE CONJUGATES

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Modern synthetic design demands high efficiency in terms of minimization of synthetic steps together with maximization of complexity. efficiency and utility of a tandem reaction can be measured in terms of the number of bonds formed in the overall sequence, the degree of increase in the structural complexity and its applicability to broader classes of substrates. The main benefits of tandem reaction include high atom economy and reduction of waste, time.[1] Medicinal chemists have considered the synthesis of 1, 2, 3-triazole based heterocycles as the corner stone of medicinal chemistry due to their important biological activities. Triazole based compounds exhibits antitubercular, antibacterial, antiallergic, anti- (HIV), antifungal and α-glycosidase inhibitor activity [2]. Pyrazole and its derivatives are significant because of their wide spectrum of biological activities and their presence in naturally occurring compounds[3]. Synthesis of triazole linked heterocyclic scaffold has been focused in order to enhance activity of target drug molecule.

Therefore, a series of novel 1, 2, 3-Triazole linked Pyrazole derivatives were synthesized via tandem reaction in good to excellent yields and will be presented.

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P-128

In planta characterization of sterol 22-desaturase (CYP710A1) from *Withaniasomnifera* in heterologous host (*Nicotiana tabacum*)

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Abstract: *Withania somnifera*is ahighly valuable medicinal plant, synthesizing a wide array of pharmacologically dynamic compounds known as withanolides. Despite their remarkable biological versatility, their biosynthetic pathway remains yet to be fully elucidated. In the withanolide biosynthetic pathway, most of the downstream reactions are catalyzed by cytochrome P450s. In the present study, sterol 22-desaturase (*Ws*CYP710A), a cytochrome P450 was isolated from *Withania somnifera*.The full length cDNA of *Ws*CYP710A1 contained an open reading frame of 1530 bp corresponding to 506 amino-acids.Further,over-expression of *Ws*CYP710A1 in hairy roots showed a significant enhancement of mRNA level coincident with enhanced withanolide accumulation. Furthermore, two allelic isoforms of *Ws*CYP710A1 in hairy roots were confirmed by using southern blot analysis. Additionally, *in planta*,characterization of *Ws*CYP710A1in *Nicotiana tabacum*was carried out. Transgenic lines were established which were confirmed via semi-quantitative and quantitative real time PCR analysis. HPLC demonstration showed 3-fold increase in the sterol contents in transgenic lines compared to control.Present study is so far the only report of molecular characterization, functional validation and *in planta* characterization of *Ws*CYP710A1 from *W.somnifera*.

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Enzyme inhibitors unravel precursor diversion via non-mevalonate pathway for intensified camptothecin biosynthesis in *Nothapodytes nimmoniana*

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Abstract: *Nothapodytes nimmoniana* is an important medicinal plant well known for camptothecin (CPT) production. It is a monoterpene indole alkaloid (MIA), having robust anti-microbial, anti-viral and anti-tumor activities. However, no substantial progress has been made related to biosynthetic and regulatory mechanism of CPT, presumably because of the lack of genomic resource and *in vitro* experimental mode. In the present study, an efficient *in vitro* regeneration system via forced axillary bud induction and *Agrobacterium rhizogenes* mediated hairy root induction protocol was developed. Further, two important enzymes 1-deoxy-D-xylulose-5-phosphate reductoisomerase (DXPR) and 3-hydroxyl-3-methylglutaryl-CoA reductase (HMG) of methylerythritol 4-phosphate (MEP) and mevalonate (MVA) pathway respectively were subdued with two pathway specific inhibitors to determine the major source of monoterpene moiety in CPT biosynthesis. As a response to fosmidomycin treatment, drastic reduction of CPT accumulation around 83-91% was observed as compared to control. On the other hand 9-14% decline was observed in CPT accumulation in presence of lovastatin. Therefore, a strong reduction in CPT content via fosmidomycin treatment suggested the major role of MEP pathway in CPT biosynthesis. Additionally, quantitative real-time PCR (qRT-PCR) analysis of MEP (DXPR, DPCMEK, HMBEDPR, MECDPS) and MVA (HMG, MK, PMK, DPMD) pathway genes showed an insignificant drop in their transcript levels. An efficient *in vitro* regeneration system and transformation protocol thus developed provides a fresh perspective for biotechnological interventions in *N.nimmoniana* towards enhanced CPT production. Moreover, MEP pathway identified as major route for CPT biosynthesis may have potential implication towards metabolic engineering of CPT biosynthesis.

P-130

Design and Synthesis of π-Conjugated Fluorescent Arenes and Heteroarenes for Mechanochromic and Chemosensing Applications

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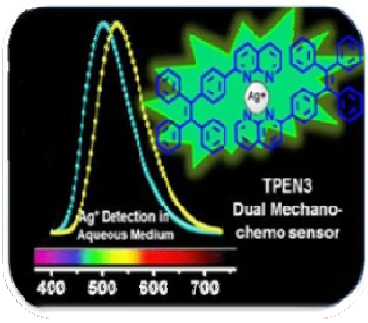
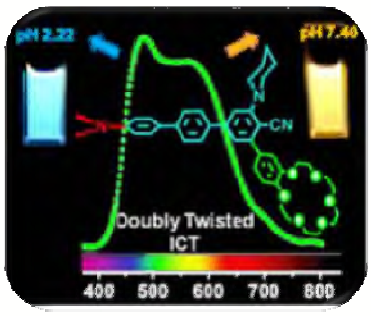
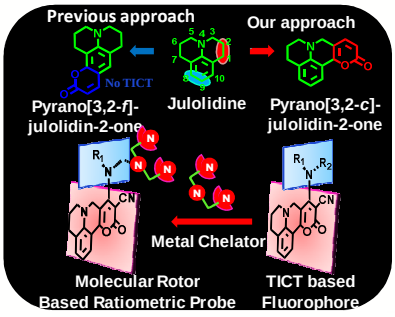
Fluorescent organic molecules play an important role in chemical and biological sciences. Fluorescent organic molecules as chemosensors have been widely applied in diverse fields such as biology, physiology, medicine, and pharmacology, as the variations of fluorescence signals can be observed through optical instruments and even by the naked eye in real-time. [1] Metal ions play an important role in biological system in regulation of enzymes, membrane potential and working of proteins e.g. Zn^{2+} In carbonic anhydrase and Fe^{2+} in hemoglobin. So imaging and analytical quantification of metal ions in biological system is of great importance.

In our laboratory we are engaged in design and synthesis of ICT, TICT, DT-ICT and AIE based new donor-acceptor based □-conjugated fluorescent organic molecules with variety of excitation and emission wavelength and their application in biological chemo-sensing and material sciences. [2-7] In this poster, the design and rapid synthesis of a new series of donar accepter based arenes and heteroarenes and their exciting applications in selective fluorescence imaging and sensing of metal ions will be presented in detail.

Mechanochromic and Chemosensor	pH Sensor	Hg^{2+} Sensor
		
J. Org. Chem., **2017**, *82*, 4766.	*Asian J. Org. Chem.*, **2016**, *5*, 187.	*J. Mater. Chem. B.*, **2016**, *4*, 4934.

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P-131

Novel Drug design and Inhibition of MCF-7 Breast cancer cell line, anticoagulant activities of Imidazolidine-2,4-dione, and 2-Thioxoimidazolidin-4-one Derivatives

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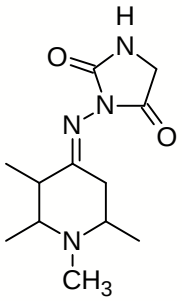
In this research, to investigate and characterization of some imidazolidine-2,4-dione, 2-thioxoimidazolidin-4-one derivatives. The synthesized compounds were confirmed by Fourier transform infrared spectroscopy (IR), proton nuclear magnetic resonance (^{1}H-NMR), carbon nuclear magnetic resonance (^{13}C-NMR), 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-methoxy phenyl)-1,3-dimethylpiperidin-4-ylideneamino)-2-thioxoimidazolidin-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.



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P-132

Effect of sodium cholate on the micellization, gelation and encapsulation behavior of Pluronic P123.

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Abstract: The effect of Sodium Cholate (NaC) on the micellization and gelation characteristics of Pluronic P123 in aqueous media have been explored using tensiometry, rheology, Dynamic light scattering (DLS), and densitometry. The aggregation characteristics were delayed drastically with the addition of NaC as signified by increase in critical micelle concentration (CMC), critical micellization temperature (CMT) and critical gelation temperature (CGT). The results were explained on the basis of electrostatic and steric destabilization of P123 micelles by cholate. The apparent hydrodynamic diameter (D_H) of P123+NaC binary systems decreased upon addition of NaCupto 1.5wt%. Further, in addition to an increase in D_H , presence of two types of scattering species was also evidenced with increase in NaC concentration from 2.5-10wt%. The effect of NaC on the encapsulating capacity of P123 was also studied using naproxen and pyrene as two model hydrophobes. The work could give a sound understanding of the interaction and self-assembling behavior of Pluronics with the important physiological component i.e, bile salts which is important to consider in any pharmaceutical formulation involving Pluronics as drug delivery agent.

P-133

Synthesis of New Cytotoxic Hybrid Molecules based on Multi-target Drug Design Approach using Combretastatin A-4 as Scaffold

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Abstract

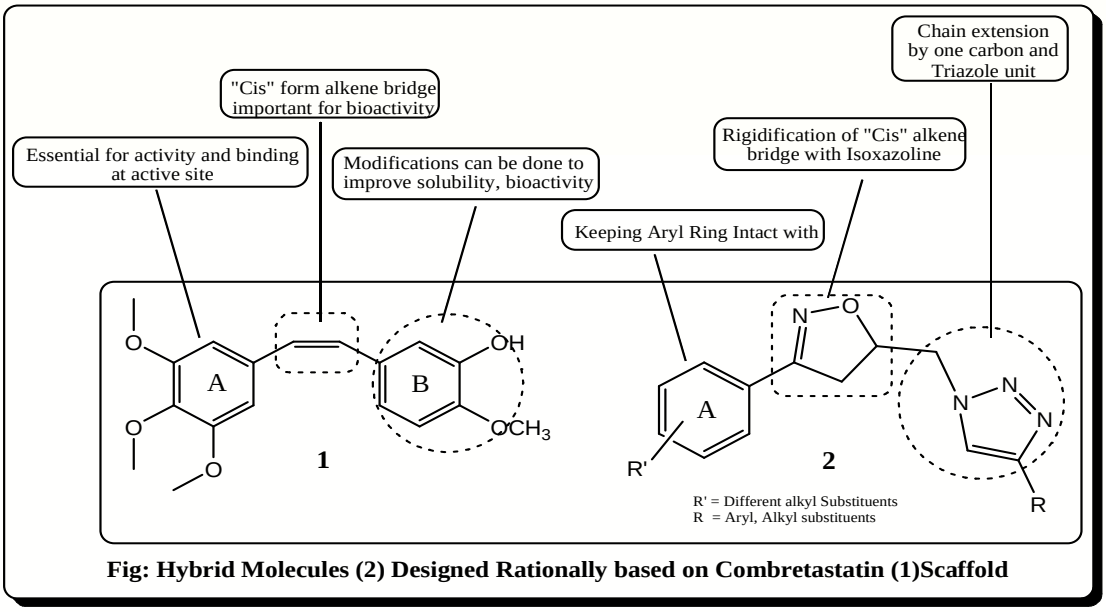

Fig: Hybrid Molecules (2) Designed Rationally based on Combretastatin (1)Scaffold

Combretastatin A-4is naturally isolated compound from *Combretumcaffrum*, a South African bushwillow tree, known for its potent anticancer activity via tubulin polymerization inhibition and antiangiogenic effects[1,2].This molecule has to still overcome hurdles like its poor solubility issue and possible conversion to less active structural *trans*- form *in vivo*,to be marketed as ananti- cancer drug[2,3].A hybrid molecule approach is enacted to improve upon these demerits and to probe more active derivatives with more than one receptor target[4].Several derivatives have been synthesized with isoxazoline ring replacing the *cis* alkene bridge from the parent Combretastatin-A4 and, replacement of Aryl ring B from the parent Combretastatin A4 by single carbon chain extended rigid triazolemoieties[3]. Replacement by isoxazoline ring will rigidify the shape of molecule (may enhance apoptotic effect) while introduction of single carbon chain extended triazolemoiety is anticipated to induce anti-angiogenic effectalso will enhance its solubility. Synthetic studies, molecular docking studies and preliminary cytotoxic studies on cancer cell lines will be presented.

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P-134

Domino ring opening cyclisation of aziridines and epoxides with nitrones via dual catalysis on water

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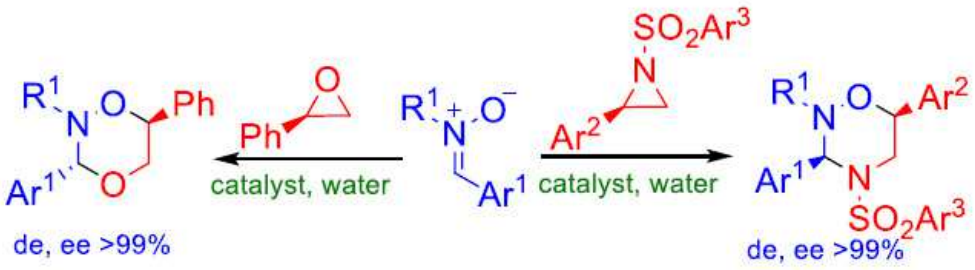
Abstract:



An efficient and green ‘‘on water’’ regio- and stereoselective synthetic route to chiral 1,2,4-oxadiazinanes and 1,4,2-dioxazinanes with excellent yields (up to 99%) and de/ee (499%) has been developed for the first time via the domino ring-opening cyclization (DROC) of *N*-activated aziridines and epoxides with nitrones using LiClO4/Bu4NBF4 a dual catalyst system. The developed green strategy features a broader substrate scope and mild reaction conditions, and successfully overcomes the competitive oxidative ring opening of aziridines. Further synthetic significances of this green protocol are the formation of the products (i) as single diastereomers starting from a mixture of cis/trans disubstituted aziridines via dynamic kinetic epimerization (DKE) and (ii) via a multicomponent approach starting from *N*-methylhydroxylamine hydrochloride, benzaldehyde and aziridine.

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2. " A Synthetic Route to Chiral 1,4-Disubstituted Tetrahydro-β-Carbolines via Domino Ring-Opening Cyclization of Activated Aziridines with 2-Vinylindoles" Masthanvali Sayyad, Abhijit Mal, **Imtiyaz Ahmad Wani,** Manas K. Ghorai**.** *J. Org. Chem.* **2017**, *82*, 2364-2374.

P-135

Tumor Necrosis Factor-alpha inhibitory activity of *Halodule pinifolia*

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Halodule pinifolia (Family: Cymodoceaceae) is a common sea grass found from Bay of Bengal to Coromandel Coast of India. *H. pinifolia* possessing antioxidant and antibacterial properties along with nutritional values was tested for its inhibition potential against the major pro-inflammatory cytokine TNF-α in RAW 264.7 cells using ELISA kits. The dry methanolic extract (MHP) obtained by hot extraction after defatting procedure using hexane was tested at different concentrations. MHP exhibited 67.37 % inhibition of LPS-induced TNF-α at 250 µg/mL treatment (IC_{50} 225.2µg/mL). MHP was also subjected for MTT assay to assess the cytotoxicity, which demonstrated IC_{50} value of >300 µg/mL. Further the total phenolic and flavonoid content of MHP was estimated by UV-spectrophotometric method which showed 364.0 mg/g and 185.6 mg/g, respectively. The significant TNF-α inhibition effect along with weak cytotoxicity and high phenolic content explores the scope of emergence of *H. pinifolia* as an alternate medicine for inflammatory disorders.

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P-136

3D-QSAR And Molecular Docking Studies of Aminoquinoline-pyrimidine Hybrids with The Wild-type (D6) and mutant (W2) Strains of Plasmodium falciparum

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4-aminoquinoline-pyrimidine hybrids were identified as potential antimalarial agents showing substantial antiplasmodial activities in vitro against Plasmodium falciparum W2 and D6 strains. Our previous studies using molecular modelling techniques, have conclusively established that4-aminoquinoline-pyrimidine hybrids were capable in forming H-bond and hydrophobic interactions in the active site of Pf-DHFR, similar to Pf-DHFR inhibitors (cycloguanil and pyrimethamine) and native substrate dihydrofolate. Thesefindings indicatethat Pf-DHFR protein could be the possible target for 4-aminoquinoline-pyrimidine hybrids. In the present study, we have attempted to develop a quantitative structure activity relationship (QSAR) model, using series of previously synthesized aminoquinoline-pyrimidine hybrids, based on their antiplasmodial activities obtained byin vitroexperiments against the chloroquine sensitive D6 strain as well as the chloroquine resistant W2 strain. The best statistically significant QSAR model (QSAR statistics) were validated using external test set.Further, chemical features based pharmacophore models were developed using the antiplasmodial activity of 4-aminoquinoline-pyrimidine hybrids against both D6 and W2 strains using Phase module implemented in Schrödinger program suite. The constructed pharmacophore models of 4-aminoquinoline-pyrimidine hybrids were further cross-validated using test set. The best quantitative pharmacophore and QSAR modelswere cumulatively utilized to design potential compounds as Pf-DHFR inhibitors. The ADME properties of the designed compounds were predicted using QikProp descriptors (Schrödinger, LLC, New York, NY, 2012). The compounds showing favourable pharmacokinetic properties were finally docked in the Pf-DHFR active site using Glide Program (Schrödinger, LLC, New York, NY, 2012).

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P-137

PYRAZOLE INCORPORATED MONOCARBONYL CURCUMIN ANALOGUES AS ANTIPROLIFERATIVE AGENTS

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Abstract: Monocarbonyl analogue of curcumin is one of the class of structurally modified curcumin analogue which is obtained by removing β diketone moiety and active methylene group from curcumin.[1-2] In recent years, pyrazole and its derivatives emerging as one of the most biologically active class of heterocyclic compounds. Literature reveals that pyrazole containing compounds exhibit broad spectrum biological activities such as anticancer, cardiovascular, antitubercular, antimicrobial, anticonvulsant, anti-inflammatory etc. [3,4]

In present study, a series of sixteen pyrazole incorporated monocarbonyl analogues of curcumin were designed and synthesized. Some of the compounds effectively inhibited *MDA-MB-231* (human breast adenocarcinoma) and *L132* (lung adenocarcinoma) tumor cell lines proliferation in MTT assay. Furthermore, Molecular docking study carried out, which reproduces similar results of biological activity suggesting that these compounds have a potential to become lead molecules in drug discovery process.

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P-138

Glycerol as a Recyclable Solvent for Copper-Mediated Ligand-Free C-S Cross-Coupling Reaction: Application to Synthesis of Gemmacin Precursor

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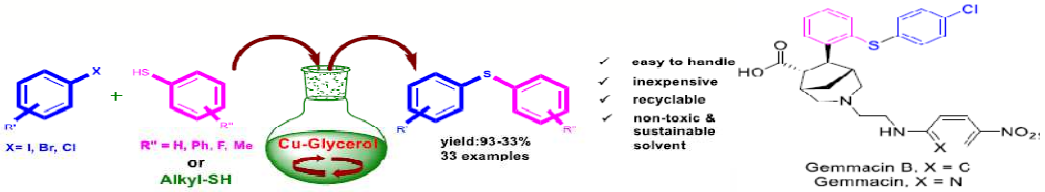
A highly efficient copper catalyzed ligand-free C-S cross-coupling reaction of aryl halides with thiols has been performed in the presence of environmentally benign solvent glycerol. A variety of diaryl and arylalkyl thioethers including the difunctional group are prepared with good chemoselectivity and functional group tolerance. The catalytic system is found to be active for more challenging, less reactive aryl bromides and chlorides. Both electron rich and deficient aryl halides including the hetero and sterically hindered ones effectively reacted to form the products in good to excellent yields. The catalyst and solvent are found to be recyclable up to five cycles. Additionally, the developed methodology is used for the synthesis of the sulfide precursor of biologically active antibiotic molecules Gemmacin B and Gemmacin.



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P-139

Layer-by-layer assembled dual imprinted polymers of acrylamide functionalised reduced graphene oxide and acrylamide functionalised fullerene on pencil graphite electrode for enantioselective differentiation of D- and L-Serine at ultra-trace level

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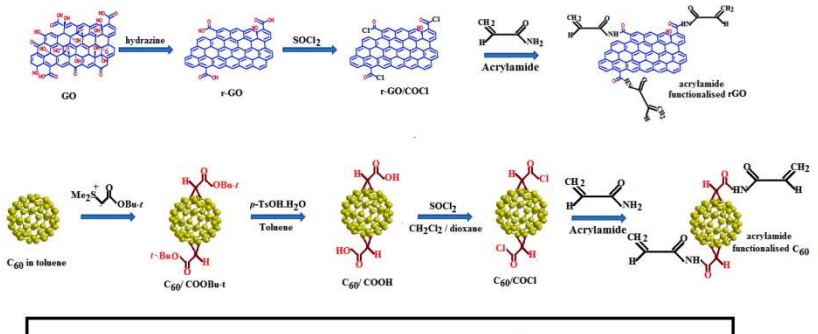
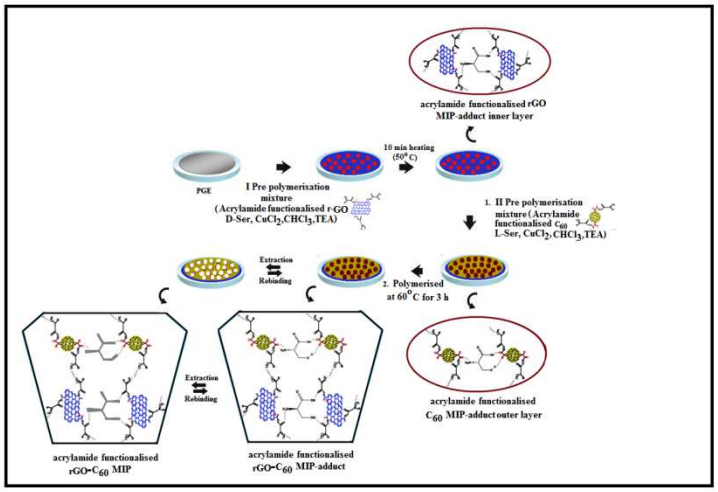
ABSTRACT: The present work describes a new, simple, and easy method for the generation of acrylamide functionalised reduced graphene oxide-fullerene layer-by-layer assembled dual imprinted polymers to quantify D- and L-Serine in aqueous and real samples. Herein, the pencil graphite electrode was initially spin coated with D-Serine imprinted acrylamide functionalized reduced graphene oxide. After 10 min thermal treatment (50^{o}C), this electrode was again modified with L-Serine imprinted acrylamide functionalized fullerene molecules. The bilayer assembly so produced was finally made thermally stable by 60^{o}C exposure for 3 h. The proposed sensor showed an improved synergism without agglomeration between layer-by-layer films on the modified electrode, with better electronic properties. We have compared this modified electrode with other modified pencil graphite electrodes like single layered acrylamide functionalised reduced graphene oxide or fullerene, single layered acrylamide functionalised reduced graphene oxide-fullerene composite and double layered acrylamide functionalised reduced graphene oxide or fullerene molecules, which yielded very inferior sensitivity due to possible agglomeration and decreased synergism. The chosen system demonstrated a very good analytical figures of merit with differential pulse anodic stripping voltammetry and cyclic voltammetry transduction, showing lower limits of detection (0.24 ng mL^{-1}, *S/N =3*) for both isomers. The proposed sensor assures practical applications as disease biomarker manifesting several diseases at very ultra-trace level.





P-140

Methylene Blue alleviates Rotenone induced mitochondrial dysfunction and cyto-toxicity by modulating mitochondrial permeability transition pore in SH-SY5Y cells

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Parkinson's Disease is a progressive neurodegenerative disorder that affects approximately 1% adults older than 60 years of age. PD is the second most common neurodegenerative disorder after Alzheimer's disease. The most common pathological feature of PD is formation of alpha synuclein inclusions named Lewy bodies. The loss of more than 80% of dopaminergic neuron population in substantia nigra leads to Parkinson's Disease like symptoms. Although, most of PD cases are related to hereditary causes, herbicides and pesticides like rotenone and paraquat have been shown to cause PD like symptoms.

In this study, we have used an in vitro toxicant based model to test the efficacy of Methylene Blue (MB), an antioxidant, against Rotenone induced mitochondrial dysfunction, consquent oxidative stress and cell death in SH-SY5Y neuroblastoma cell line. We observed that treatment with MB (0.5 µM and 1 µM) alleviated the toxicity caused by Rotenone (100 µM and 200 µM) in a dose dependent manner. Our results also indicated that restoration of mitchondrial membrane potential and modulation of mitochondrial permeability transition pore (mPTP) is involved in the protective function of MB against Rotenone cytotoxicity. Based on these results, further exploration of protective efficacy of MB can lead to new avenues of therapy of PD and better understanding of the disease in general.

Keywords: mPTP, apoptosis, mitochondrial dysfunction, Parkinson's Disease

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CONFIRMATIONS OF VICINAL DISULFIDE BOND IN PEPTIDES AND PROTEINS

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Vicinal cysteine disulfide, the disulfide between adjacent cysteine residues in the sequences, is the rare conformation of peptides and proteins. Structures of large number of vicinal disulfide containing proteins including enzymes, peptide toxins and channel/ receptors are deposited in PDB. We have made attempt to characterize the conformational features of vicinal disulfides in the available X- ray structures of peptide and proteins. We have used back bone torsional angles,Cα /Cβ distances, backbone dihedral angles and disulfide strain energy as a probe for conformational analysis of vicinal disulfide. We have analyzed conformational feature using publically available software such as disulfide strain energy server ChemBio 3D ultra and Ramachandran map 2 to collect the parameters of vicinal disulfides. Total 103 vicinal disulfides containing proteins are retrievedfrom PDB. Analysis of side chain torsional angle of cysteine disulfide revealed presence of following conformations in vicinal disulfides: (+,-) LH staple, next is (-,-) RH staple, Anti LH hook, (+,-) Anti RH hook, (+,-) RH staple, (-,-) LH staple, (+, +) RH staple. Measurement of Cα/Cα and Cβ/Cβ distances of cysteine revealed high value of Cβ-Cβ over Cα–Cα which is against the conventional features of disulfide in peptide and proteins. Calculation of disulfide strain energy reveals less stability of some of the vicinal disulfide conformers which are actually preceded by the Proline residue in the sequence.The back bone torsional angles of vicinal disulfides were further probed using Ramachandran map. Analysis of conformational features of vicinal disulfides assisted to identify redox peptide motif which can act as good oxidizing agent for oxidative protein folding.

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P-142

Biophysical Studies on Deoxyribose-Glycated Whole Histone

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Reactions of reducing sugars with free amino groups of proteins can form advanced glycation end products (AGEs). AGEs can interfere with the proper functioning of the proteins to which they are attached. As such, non-enzymatic damage to nuclear proteins has potentially severe consequences for the maintenance of genomic integrity. The nucleosome is comprised of an octamer of two copies each of H2A, H2B, H3 and H4 histones and 146bp DNA. Histones have a central structural and epigenetic role in mediating gene expression as well as various metabolic functions such as maintenance of chromosomal integrity and the process of DNA replication itself. Recent studies have shown that histones are highly susceptible to non enzymatic glycation and oxidation, leading to the irreversible formation of pathogenic AGEs.

In the following study, commercial whole histone preparations were glycated using deoxyribose and the biophysical changes were analysed using UV and fluorescence spectrophotometry. The hyperchromicity of modified histone shown in the UV spectral profile and increased intensity of AGE-specific fluorescence indicate the formation of advanced glycation end products (AGEs). The elevated levels of amadori adducts on the 4th day of incubation indicates the formation early glycation products, while the increased carbonyl content, being a marker for oxidative stress, is suggestive of AGE formation in the deoxyribose-glycated histone. Changes in secondary structure were revealed by the shift in peak positions in FT-IR spectroscopy.

The results so far indicate that glycation of whole histone with deoxyribose leads to major structural changes in the protein. These modified proteins may be involved in initiating the immune response in autoimmune diseases like SLE, playing a role in the pathogenesis of the disease.

Keywords: glycation, histone, deoxyribose, AGEs, SLE

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In Silico Docking to elucidate Interface the effect of Plant-Originated Inhibitors and L1 capsid Protein of Highly Threatening Human Papillomavirus 11

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Cervical cancer is a type of cancer that develops in a woman's cervix . The principle cause of cancer mortality worldwide amongst the women is due to human papillomavirus (HPV) infection. There is urgent need to discover anti-cancerous drugs against this life-threatening infection. Natural compounds are hopeful source of cancer treatment. In the present study, we explored 3071 natural compounds against L1capsid protein of high risk HPV11, which is known to protect HPV inside the host. Vaccines that contain virus-like particles (VLPs) made of L1 capsid protein from several high risk HPV types have proven to be effective against HPV infections. L1 capsid protein (2R5K) X ray crystallographic protein model , was predicted to anticipate the interaction mechanism with these natural inhibitors using structure-based drug designing approach using Discovery studio 3.5 and Autodock. Docking analysis showed the interaction of 16 natural inhibitors with binding site of L1 protein residues, docking analysis besides helping *in silico* validations of natural compounds also helped elucidating the molecular mechanism of inhibition of HPV oncoproteins.

Keywords: Human papillomavirus 11, molecular docking, natural compounds and Discovery studio3.5

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ZYMOGRAPHY (*IN-GEL* ASSAY): A MODIFIED TOOL FOR MONITORING MUSCLE SPECIFIC NATIVE CALPAIN ACTIVITY

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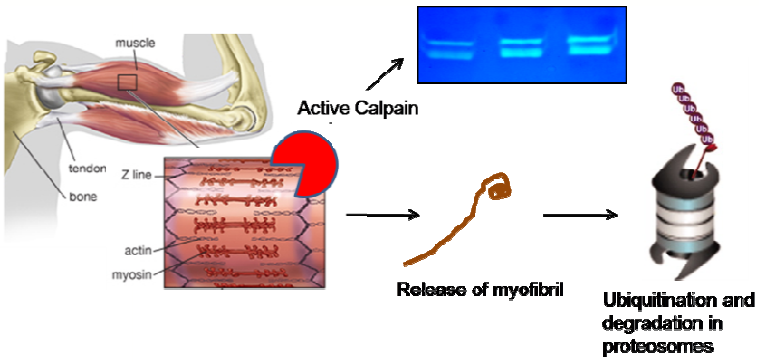
Abstract: Proteostasis is a critical factor in avoiding the onset and progression of many cellular dysfunction including muscles related disorders. Unregulated proteolysis is generally associated with the pathological conditions and is a principle mechanism behind skeletal muscle atrophy. Despite the negative connotation of proteolysis its long-term association during organ development (say muscle formation) and proper functioning cannot be ignored. Thus, clear vision of different proteolytic enzymes is gaining attention in the health issue associated with muscles. It is a critical organ constantly affected by different kinds of challenges such as oxidative and inflammatory stress (during exercise, aging, and diseases), mechanical stress and thermal stress. Calpain is a proteolytic enzyme, playing important role in skeletal muscle patho-physiology and thus can be the potential therapeutic target under regenerative medicines. Easy detection of calpain at very early stage will be helpful in understanding muscle protein metabolism well in time. Multiple methods are available (zymography, qPCR and immunoblotting) and among these zymography is the only approach which mark the active state of this enzyme. In the present study, we have developed efficient and modified zymography protocol(s) which are able to detect calpain in all muscle cells/tissues. The calpain data produced using these methodologies were compared with other reported protocols. Our approach have tremendously improved the quality of calpain activity even at low protein concentration (5 □g) in muscle cells (C2C12 myoblasts; myotubes) and tissues (cardiac/ skeletal) in a single gel in comparatively short time span. Overall, the present paper provide relatively simple, authentic and well described experimental protocol which can be used for muscle-specific calpain study [1].



Key Words: Calpain, Muscle, Zymography

Reference:

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P-145

CiNA AS A PHYTOAGENT FOR AN UNRESOLVED HEALTH ISSUE- SKELETAL MUSCLE ATROPHY

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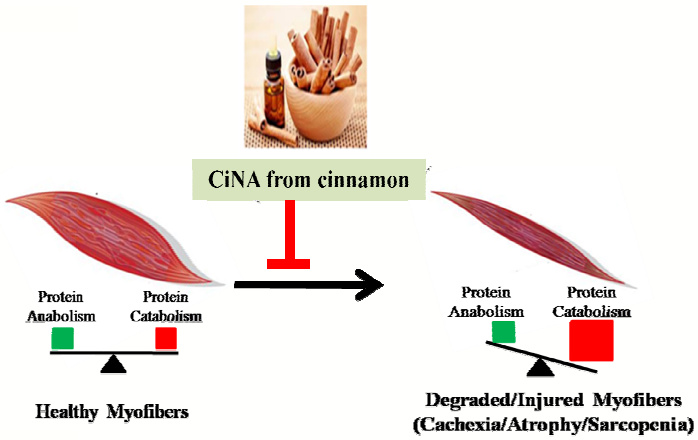
Abstract: Skeletal muscle atrophy (characterized by loss of muscular mass) is associated not only with physical capacity impairment under physiological conditions (starvation, inactivity/space flight and aging) but also a key factor behind the increasing rate of mortality in diverse pathophysiological conditions (cancer, COPD, AIDS). Despite the success in revealing the in-depth mechanisms, the recommended therapy/drug against atrophy/cachexia in such pathological conditions is still a dream [1]. Thus, there is a necessasity to explore such compound(s) which can have multi-targeted approach to obstruct or prevent its origin. Integration of botanicals has provided a wide vision for obtaining a potent bioactive agent for various deadiler diseases. One such compound CiNA present abundantly in cinnamon (*daalchinni*) has been documented to possess wide spectrum of pharmacological properties including anti-inflammatory in various clinical stettings as it inhibits the level of inflammation. But its role as an anti-atrophic agent is unknown. We hypothesize that CiNA may be the potential candidate to combat inflammatory stress-induced atrophy.



In this direction we established atrophic conditions with the help of pro-inflammatory cytokine (TNF-α) in C2C12 cultured myotubes and explored the potential of CiNA by using real-time PCR, western blot, Immuno-florescence staining tools. Current findings provide a strong evidence for emergence of CiNA as an anti-atrophic agent as it remarkably ameliorated the up-regulated protoelytic machinery and inflammatory marker molecules simultaneously with improved muscle morphological parameters such as myotube length and diameter in atrophic prone envirnment.

Key Words: CiNA, Phyto-compound, Skeletal Muscle Atrophy, Proteolysis, Inflammation

Reference:

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P-146

Design and synthesis of 1,2,3-triazolyl sulfonyl analogues as anti-tubercular agents

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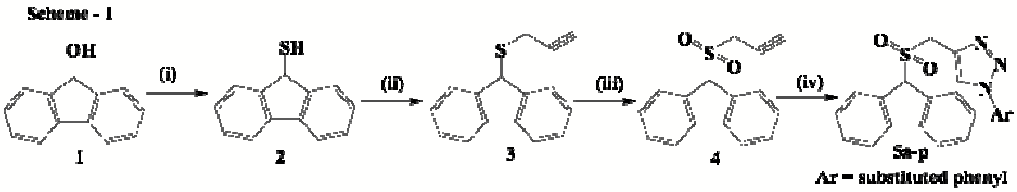
We designed and synthesized sixteen various 1,2,3-triazolyl sulfonyl analogues using click chemistry. The target compounds were characterized by routine analytical techniques *viz.*,^{1}H, ^{13}CNMR, Mass, Elemental, and screened for *in vitro* antitubercular activity against *Mycobacterium tuberculosis* (MTB) H37Rv strain and two 'wild' strains *Spec. 210* and *Spec. 192* and MIC_{50} was determined. [1] The final analogues exhibited minimum inhibitory concentration ranging from 52.35 - > 258.09 µM. We synthesized 4-(((9*H*-fluoren-9-yl)sulfonyl)methyl)-1-substituted phenyl-1*H*-1,2,3-triazole, analogues as sketched in **Scheme-1**. We adopted reported procedure with slight modification to prepare target molecules **5a-p**. [2-3] All the synthesized derivatives were tested for their capacity to inhibit the growth of MTB against the three different strains (MTB H37Rv, MTB *spec. 192*& MTB *spec. 210*). **5p** with three methoxy groups emerged to be the most active compound among these sixteen derivatives with MIC 52.35 µM. Further, **5p** was found to be non-cytotoxic against HEK 293 cell lines at 50 µM (**Figure-1**). Structure activity relationship is explained with respect to **5a** which showed MIC 258.09 µM. Activity increased by more than two folds with electron donating 4-methyl, 4-ethyl and 4-methoxy (MIC 124.53, 120.33 and 119.76 µM respectively). Among the halo derivatives, activity remained unaltered with bromo where as it increased by two folds with 4-flouro and 4-chloro derivatives. Electron withdrawing NO_2 at second & fourth positions did not impact the activity; with electron withdrawing disubstituted derivatives activity remained unaltered (**5m, 5n**& **5o**). Presence of electron donating dimethyl increased the activity by two folds (**5l,** MIC 120.33 µM).



Reagents and conditions: (i) Lawesson reagent (2.0 eq), toluene, 110 °C, 16 h. (ii) Propargyl bromide (2.0 eq), TEA (3.0 eq), DCM, 16 h. (iii) *m*-CPBA(2.0 eq), DCM, 2h. (iv) Substituted aromatic azides, $CuSO_4.5H_2O$ (10 mol %), Sodium ascorbate (5 mole %), H_2O:*t*-BuOH (1:2), rt, 16 h.

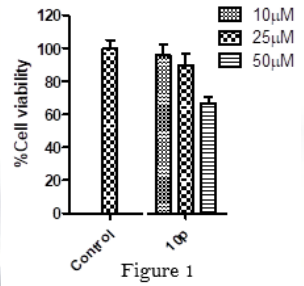


Figure 1

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P-147

Antiobesity potential of selected Indian medicinal plants: A Pancreatic Lipase Inhibition based study through synergistic approach

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Obesity is a multifactorial metabolic disorder characterised by excessive accumulation of fat in the body. Among different strategies for the treatment of obesity, pancreatic lipase (PL) is considered as successful target. PL is adigestive enzyme responsible for the breakdown of fats (around 60-70%) in to monoglycerides. Orlistat is the only drug approved for the treatment of obesity through inhibition of PL,thatwas found to exertsevere adverse effects like hepatotoxicity, renal failureetc.on long term treatmentFDA report [1].Currently, synergy based treatment approach is gaining more interestwherein the dose of the individual drug is reduced while maintaining/ improving the overall efficacy. With a huge success of natural products for the management of obesity, more researchis focused on the identification of newer PL inhibitorswith lesser adverse effectsSeyedan *etal*[2]. Based on theantiobesity potential reported in *Ayurvedic* literatures, wepicked a pool of Indian medicinal plantsthat include*Curcuma longa*(rhizomes), *Garcinia indica*(fruits), *Piper longum*(fruits), *Cuminum cyminium* (fruits) and *Tribulus terrestris*(fruits) Chandrasekaran *et al*[3].The synergistic potential of the selected plants was screened in combintion with orlistat through synergy guided pancreatic lipase inhibition assay.Hexane and methanolic extracts of *C. longa* exhibitedpotent synergistic activity (IC_{50} value of 0.63 ± 0.02 and 0.61 ± 0.03, respectively)while lowering the dose of orlistat by 2.8 and 0.9-fold respectively. Further studies are required to identify the components of theseextracts which produced the synergistic activity with orlistat.

Key Words: Obesity, Pancreatic Lipase, Orlistat, Natural products, Synergy

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P-148

Electrochemical simultaneous analysis of dopamine and epinephrine using double imprinted One MoNomer acryloylated graphene oxide-carbon black composite polymer

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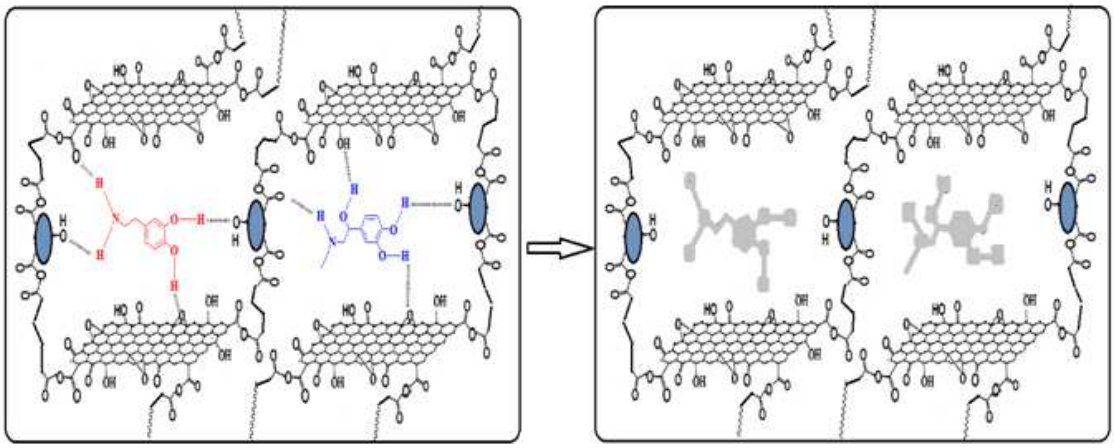
A novel One MoNomer dual imprinted graphene oxide/carbon black composite polymer was developed applying 'surface-grafting from' approach on the screen printed carbon electrode for the electrochemical sensing of dopamine and epinephrine. The oxidation peak potentials of both the targets were found separated by 200 mV which enabled their simultaneous analysis in real world samples, without any cross reactivity, interferences, and false-positives. The detection limits realized by the proposed sensor, under optimized analytical conditions, were found to be as low as 0.028, 0.028, 0.061 and 0.029 ng mL^{-1} for dopamine and 0.017, 0.018, 0.019 and 0.020 ng mL^{-1} for epinephrine (S/N=3) in aqueous, blood serum, urine and pharmaceutical samples. Such sensor could be considered suitable for the primitive diagnosis of several chronic diseases, manifested at ultra-trace level.



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MICROWAVE ASSISTED SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL ASPECTS OF HETEROBIMETALLIC COMPLEXES OF COPPER

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Abstract: The elevation in the field of bioinorganic chemistry has led to the use of metal complexes due to their imperative applications for the development of advanced novel technologies which includes chemotherapeutic and diagnostic devices. In recent years, studies of heteronuclear bimetallic complexes havebeen of cumulative importance in inorganic and bioinorganic chemistry. The presence of two metals in the same molecule largely affects both the physical properties and the reactivity of the complexes**.**In this communication we have made an attempt to synthesize heterobimetallic complexesof copper using microwave radiations.Microwave-assisted synthesis is considered to be a promising green chemical approach because it reduces reaction time from days or hours to minutes or even seconds.Microwave is a convenient way toward the goal of green/sustainable chemistry offering many advantages. For this reason, microwave irradiation is presently seeing an exponential escalation as compared to conventional methods which entail more reaction time and drastic conditions of temperature.These synthesized complexes are characterized by physicochemical and spectroscopic techniques such as IR, mass and ESR spectra. These complexes have been further screened for their antifungal, antibacterial and anti-inflammatory effects and the results are then compared with the starting materials.

Key Words*: Heterobimetallic, Microwave-assisted, Antifungal, Antibacterial and Anti- inflammatory effects.*

P-150

NATURAL PROLINE-RICH CYCLOPOLYPEPTIDES FROM MARINE ORGANISMS: CHEMISTRY, SYNTHETIC METHODOLOGIES AND BIOLOGICAL STATUS

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ABSTRACT: Peptides have gained increased interest as therapeutics during recent years. More than 60 peptide drugs have reached the market for the benefit of patients and several hundreds of novel therapeutic peptides are in preclinical and clinical development. The key contributor to this success is the potent and specific, yet safe, mode of action of peptides. Among the wide range of biologically-active peptides, naturally-occurring marine-derived cyclopolypeptides exhibit a broad range of unusual and potent pharmacological activities. Because of their size and complexity, proline-rich cyclic peptides (PRCPs) occupy a crucial chemical space in drug discovery that may provide useful scaffolds for modulating more challenging biological targets, such as protein-protein interactions and allosteric binding sites. Diverse pharmacological activities of natural cyclic peptides from marine sponges, tunicates and cyanobacteria have encouraged efforts to develop cyclic peptides with well-known synthetic methods, including solid-phase and solution-phase techniques of peptide synthesis. The present review highlights the natural resources, unique structural features and the most relevant biological properties of proline-rich peptides of marine-origin, focusing on the potential therapeutic role that the PRCPs may play as a promising source of new peptide-based novel drugs.

KEYWORDS: proline-rich cyclic peptide; marine sponge; marine tunicate; peptide synthesis; stereochemistry; lipophilicity parameter; pharmacological activity.

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P-151

Flavonoid glycosides from holy basil (O*cimum sanctum l. family Lamiaceae*) leaves improve redox status of human lymphocytes under induced oxidative stress

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Abstract: Proliferating industrialization, increasing pollution, lethargic life style and socio-economic status are related to the development of various acute and chronic pathological conditions. Lymphocytes, the instrumental cells of the human immune system are exposed to high and long standing oxidative stress generated under pathological conditions. Managing the redox status of the cells, protecting antioxidant defense enzyme system can help in prevention and treatment of these diseases. Leaves of Holy Basil (*Ocimum sanctum L. Family Lamiaceae*) are traditionally used to improve immunity. The aim of the present study was to investigate the modulatory effects of the flavonoid glycosides from Holy Basil (*Ocimum sanctum L. Family Lamiaceae*) leaves on the antioxidant defense system of human lymphocytes. Culture of lymphocytes with H_2O_2 (100-250µM) in the culture medium resulted in decreased cell viability and reduced glutathione level. Increased MDA level was observed with increased GST and LDH activity.Inclusion of 8CβD glucopyranosylLuteolin, 7CβD glucopyranosylLuteolin,7CβD glucopyranosylApigenin and 6,8CβD glucopyranosylApigeninisolated from Holy Basil leaf extract could prevent H2O2 induced decline in cell viability and reduced glutathione level in a dose dependent manner. Rise in MDA level, increased GST and LDH activity observed under oxidative stress is also prevented upon pretreatment of lymphocytes with flavonoid glycoside suggesting the possible role these flavonoid glycosides can play to control the detrimental influence of oxidative stress in human lymphocytes.

Key words: Holy basil, Human lymphocytes, Oxidative stress

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One-Pot, Four-Component Synthesis and SAR Studies of New Spiro[pyrimido[5,4-b]quinoline-10,5'-pyrrolo[2,3-d]pyrimidine] Derivatives Catalyzed by β-cyclodextrin in Water as Potential Anticancer Agents

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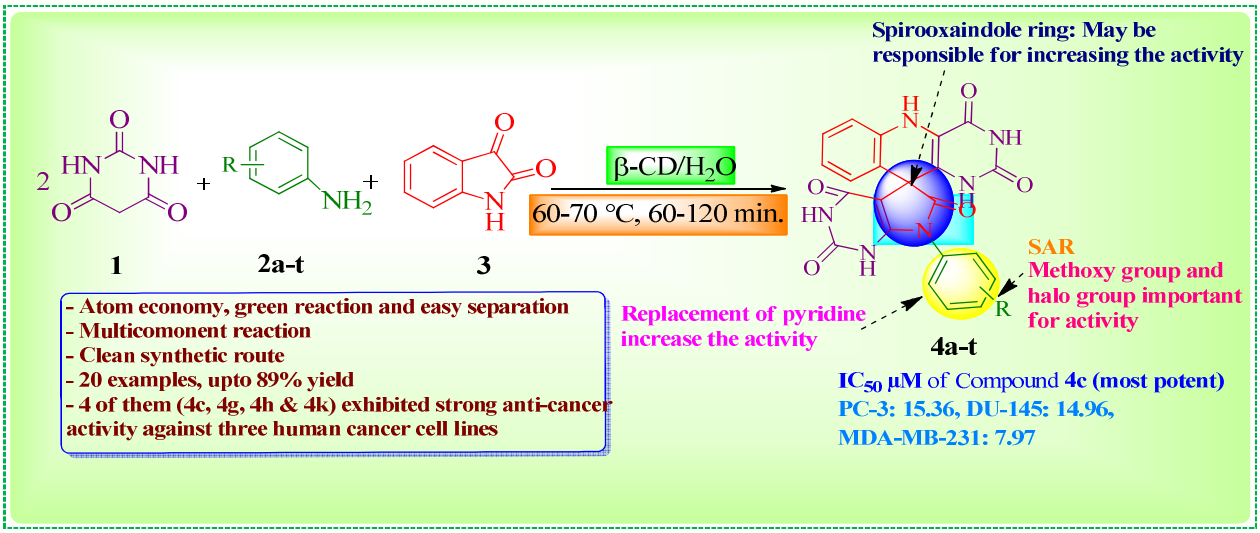

The spirooxindole system is the core structure of a variety of medicinal agents and natural products.[1,2] In fact, spirooxindole derivatives have been described with different biological activities, ranging from anti-tumor, antimicrobial, anti-HIV, antipyretics agents to sodium channel blockers and antimalarials and protein kinase B/Akt inhibitory activity useful for the treatment of cancer. [3] On the other hand, a large number of pyrimidine derivatives consist of barbituric acid have attracted great interest for their biological activities and applications in medicine and therapeutics. [2] In this context, the synthesis of this important ring system fused with spirooxindole remains a topic of current interest. The resulting pharmacological significance in compounds, which belongs to the spirooxindole family, has led us to develop the synthesis of some novel spiropyrimidines. In this work, we developed a new green protocol which is efficient and environmental benign catalyst β-CD for the synthesis novel hybrid spiro[pyrimido[5,4-b]quinoline-10,5'-pyrrolo[2,3-d]pyrimidine] derivatives.

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P-153

Synthesis, characterization and antiinflammatory evaluation of metal complexes with isoquinolone derivatives

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ABSTRACT: Metal complexes acquired a number of advantages that render them as attractive alternatives to organic small molecules for the development of therapeutic agents. In the past few decades, the research work was focused on the development of metal complexes for the treatment of inflammatory. In the present study, the anti-inflammatory activity of the metal complexes of isoquinolone analogs has been studied using the carrageenan induced hind paw oedema method in albino rats. The metal(II) ions with the bioactive ligands (derived from isoquinolone analogs (formed by the condensation of 2H-isoquinolin-1-one with 4-chloroaniline followed by 2-hydroxybenzaldehyde). They were characterized using analytical data, FT-IR, electronic spectra and mass spectral studies. The ligands behave as bidentate nature. The antibacterial activities and anti-inflammatory activities were evaluated by the agar well diffusion method and carrageenan-induced hind paw edema method, respectively. All the synthesised compounds showed considerable antibacterial activities and moderate anti-inflammatory activities as compared to ibuprofen. The obtained results showed that the most active compounds could be useful as a template for future design, modification and investigation to produce more active analogs.

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Synthesis, characterization and antituberculosis evaluation copper complexes of flavone derivatives

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ABSTRACT: In the present study, a series of novel flavone derivatives and their copper complexes were synthesized. All the copper complexes were characterized by elemental analyses, electronic, IR, NMR, mass and ESR spectroscopic techniques. The prepared copper complexes of flavone derivatives showed significant antibacterial activity against the organisms *Staphylococcus aureus, Escherichia coli and Pseudomonas aeruginosa* when compared with the standard antibiotic Streptomycin. All the complexes showed good free radical scavenging activity which is comparable to that of the standard ascorbic acid. Among these complexes, the copper complex was showed higher activity. Based on the observed results, the flavone (structural core) and copper ion could be responsible for the potential candidate eliciting antioxidant activity. All compounds were evaluated for their *in vitro* antimycobacterial activity against *Mycobacterium tuberculosis*. Anti-TB activity of the ligand has enhanced on complexation with Cu(II) ion which increases the lipid solubility. Copper complex of L^1 showed to play a key role in the antitubercular potency of new class of metal-based compounds.

Keywords: antioxidant; flavone; standard; ascorbic acid.

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COMPUTATIONAL STUDIES ON THE EFFECT OF INTRODUCING A π-BRIDGE ON THE EFFICIENCY OF A PERYLENE-BRAZILEIN BASED D-D-π-A SYSTEM

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Abstract: We report DFT studies on some perylene based dyes for their electron transfer properties in solar cell applications. The study involves modeling of donor - donor - π - acceptor type sensitizers, with perylene and brazilein as donors and thiophene as the π-bridge. The effect of introducing a π-bridge as well as varying the π-bridges in this D-D-π-A framework was evaluated in terms of opto-electronic and photovoltaic parameters such as HOMO-LUMO energy gap, λ_{max}, light harvesting efficiency(LHE), electron injection efficiency ($Ø_{inject}$), excited state dye potential (E^{dye*}), reorganization energy(λ), and free energy of dye regeneration (ΔG^{Regen}_{dye}). All quantum computations were carried out using DFT using 6-311G(d, p) / LanL2DZ (for I and Ti atoms) as the basis sets and B3LYP[1] as the functional, both in the gas phase as well as solvent phase, with Gaussian 03[2] set of codes. We found that the sensitizers exhibited good optical as well as photovoltaic response with PB2, PB7, PB8 and PB9 having benzene, pyrimidine, pyrazine and aniline as π-bridges, exhibiting better electron injection efficiencies and hence expected to be better sensitizers. The overall opto-electronic and transport parameters of the TiO_2 - dye adsorbed systems after anchoring the dyes on the model TiO_2 cluster was also studied.

Keywords: Dye sensitized solar cells: DFT: Photovoltaic response: Optoelectronic.

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Nano-Catalysed Synthesis of 3-Acetyl-2-Methyl-4,6-Diphenylpyran Derivatives

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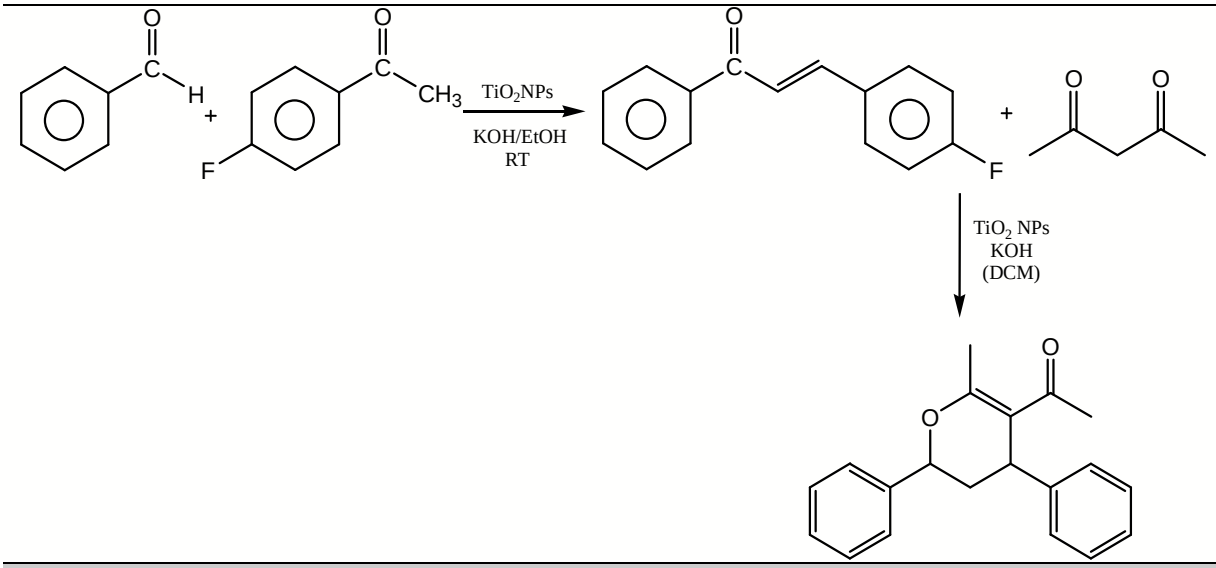
Abstract: Pyran derivatives have importance in the field of biological science as these derivatives are the part of many biologically active molecules which show antifungal, antibacterial, antiviral activities. Pyran derivatives[1] are the building units of many heterocyclic moieties like chromones,[2-3] coumarins,[4] etc. Here we are reporting the formation of 3-acetyl-2-methyl-4,6-diphenylpyran from the reaction of *α,β*-unsaturated Ketone (chalcone) and acetylacetone in the presence of nano-catalyst TiO_2 in excellent yield. The advantages of the reaction are economical profitable, short reaction time, excellent yield, recycling of catalyst, etc. The synthesized compounds are characterised by IR, ^{1}H-NMR, ^{13}C-NMR and MASS Spectrometry.



Scheme 1: **Nano-Catalysed Synthesis of 3-Acetyl-2-Methyl-4,6-Diphenylpyrane from Acetylacetone and *α,β*-Unsaturated Ketones.**

Keywords: Nano Catalysed, Synthetic Organic Chemistry, Chalcone, Biologically Active Heterocycles.

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P-157

N-Substituted 4-aminoquinoline-pyrimidinebased molecular hybrids as antiplasmodial agents

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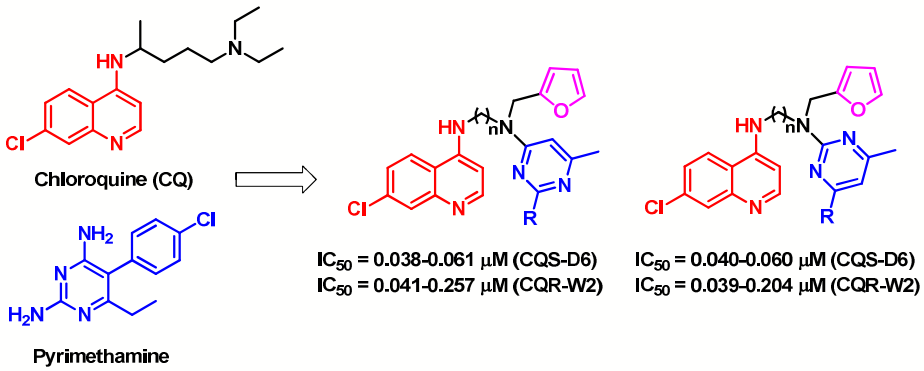
Abstract: 4-Aminoquinoline-pyrimidine based molecular hybrids with different substitution pattern in the terminal nitrogen of the linker and pyrimidine motif were designed and synthesized as antiplasmodial agent. The synthesized compounds were characterized and antiplamodial activity evaluation revealed that most of the compounds were active against both chloroquine-sensitive and chloroquine-resistant strains with high selectivity index. In order to understand safety profile of these compounds, toxicity studies was conducted against Vero cells and these compounds were found to be non-toxic upto 10 µM concentration. The most active compound was analysed for heme binding activity using UV-spectrophotometer.UV studies confirmed the interaction of the compound with heme and the binding stoichiometry between the compound and heme was found to be 1:1 by Jobs plot. Molecular docking of the most active compound was studies with wild type *Pf*-DHFR-TS and quadruple mutant *Pf*-DHFR-TS and results shows that the molecule fits well in the binding pocket of the target.



P-158

Solubilization of pyrene in anionic polymer - cationic / nonionic surfactant systems: Effect of polymer concentration

ROHI MASRAT

Abstract: Polymers may be used to alter the ability of surfactant micelles to solubilize (polycyclic aromatic hydrocarbons) PAHs depending upon polymer – surfactant interactions. The purpose of this study was to investigate the solubilization capacity of mixtures of the anionic polymer sodium carboxymethyl cellulose (NaCMC) with nonionic polyoxyethylene [10] cetyl ether (Brij56) and cationic cetyltrimethyl ammonium bromide (CTAB) surfactant micelles towards pyrene (PAH). Solubilization efficiency of these mixed systems and their comparison with individual systems has been quantified interms of the molar solubilization ratio, micelle - water partition coefficient and free energy of solubilization.While the addition of anionic polymer NaCMC accelerates the solubilization capacity of cationic CTAB micelles,that of nonionic Brij56 micelles was retarded. Moreover the Solubilization capacity of above said mixed systems gets enhanced as the polymer concentration changes from below overlap (0.5%) concentration to overlap concentration (1%).

P-159

Synthesis of β-*C*-Linked 2-Arylaminopyrimidines and β-Cyclohexenone *C*-Glycosides as H3 Receptor Antagonists

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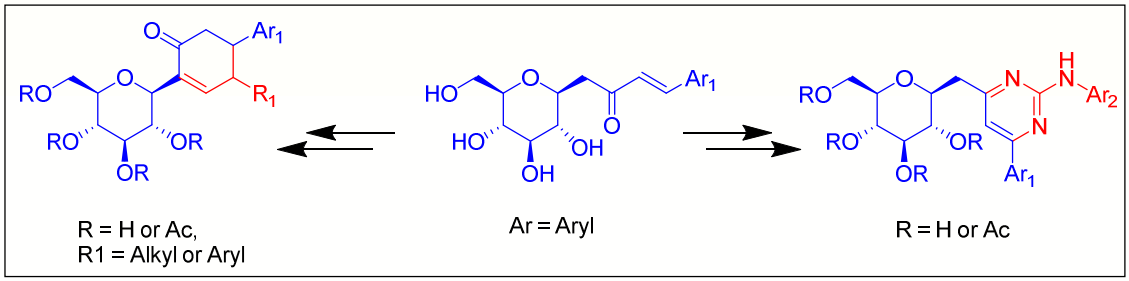

Abstract: A new series of 2-Arylaminopyrimidine and β-cyclohexenone *C*-glycosides were synthesized from *E*-butenyl-β-*C*-glucosides with polysubstituted at pyrimidine and cyclohexenone ring. The synthesized aminopyrimidine glycosides were screened for H_3R antagonist. Among all the compounds amino pyrimidine based C-glycoside proved to be potent H_3R antagonist.

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P-160

Chemically Sustainable Modified Nucleoside Synthesis and Bio-Application

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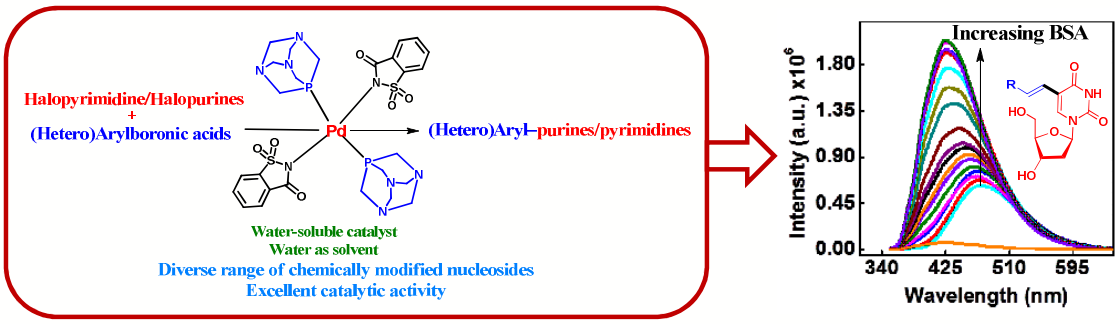
Modified nucleoside synthesis via metal-mediated cross-coupling protocol has attracted substantial attention during the last decades due to their biological applications[1].Excellent reactivity towards modification of nucleosides for suitable biological applications by Palladium complexeswith water soluble ligands have been reported.[2,3]A novel catalyst system consisting of water-soluble Pd–imidate complexes have been developed for modified nucleoside synthesis. Suzuki-Miyaura cross-coupling reaction was performed with four different nucleosides in water medium under mild conditions using the synthesized catalyst.[4]The same catalyst was also used in Heck reaction to obtain four extended fluorophoric nucleosides containing hetero or hydrocarbon aromatic moieties at the C-5 position of uridine, which were in turn mixed with different proportions with BSA. Fluorescence intensity was found to increase with increasing concentration of BSA upon excitation of the fluorophore moieties present in the nucleosides. This increase in fluorescence can be attributed to the binding of the nucleoside with BSA.



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P-161

Isolation and Structure Elucidation of Novel Oligosaccharide from Camel milk and their DFT Studies

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Oligosaccharides are the most important carbohydrate which is natural constituents of all bacteria, fungi, plants and placental mammals' milk. The milk is a rich source of oligosaccharides which have shown anti-tumor, anticancer, anticomplementary, hypoglycemic, anti-inflammatory, and anticoagulant, antiviral and immunological activities. Camel milk is used as a remedy for some diseases like tuberculosis, juvenile diabetes, liver cirrhosis, rickets, constipation, asthma, antiviral, therapeutic and antimicrobial activity. For this purpose Camel milk was collected and processed by the modified method of Kobata and Ginsburg followed by gel filtration, HPLC and column chromatography which resulted in the isolation of novel methyl oligosaccharide namely Lusoside. The HSQC spectrum of Lusoside showed four anomeric cross peaks at □□5.72 x 92.098, □□5.71 x 92.558, □□4.40 x 102.461, □ 4.42 x 102.461suggesting it to contain four monosaccharides unit which was further confirmed by ^{1}H and ^{13}C NMR of Lusoside at 400 MHz. Further the HMBC spectrum of Lusoside confirmed that the reducing glucose of compound contain a methoxy group confirming it to be a methyl tetrasaccharide. The comparision of ^{1}H and 13C NMR of Lusoside and it acetate confirmed the sequence of monosaccharides in it and position of glycosidic linkages which were confirmed by COSY, TOCSY, HSQC and HMBC and mass spectrometry. Moreover it was the first report of methyloligoglycoside isolated from any milk. The DFT studies of isolated compound were also performed. In the light of evidencees obtained from above experiments the structure of Lusoside was derived as-

α-Gal (1→4) α-GalNAc (1→4) β-Gal (1→4) β–Glc–OCH_3
LUSOSIDE

Key words- Methyloligoglycoside, camel milk, DFT, NMR.

P-162

Isolation and Structure elucidation of Buffalo milk oligosaccharide as immuno-stimulant

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Number of oligosaccharides have been isolated from various mammalian milk i.e. bear, elephant, donkey, rat, dog, cow, sheep, goat, yak and camel, which have shown anti-complementary, anti-coagulant, immune-stimulant, viral replications, parasitic infection, cell growth, cell wall adhesion and inflammation activities. Buffalo milk is also a rich source of many minerals like iron, phosphorus, sodium, zinc etc and contains riboflavin, vitamin A, C, B_6 and B_{12}. The oligosaccharides isolated from buffalo milk have anti oxidant activity and ability to stimulate non-immunological resistance of the host against parasitic infections. In our endeavor to find biologically active novel oligosaccharides, buffalo milk was taken and was processed by modified method of Kobata and Ginsburg followed by gel filtration HPLC and CC, which resulted in the isolation of one novel milk oligosaccharide namely **Eutheriose**. The structure of purified milk oligosaccharide was characterized by the combined use of chemical degradation, chemical transformation, spectroscopic techniques like ^{1}H, ^{13}C and 2D-NMR(COSY, TOCSY and HSQC) and mass spectrometry. The HSQC spectrum of acetylated Eutheriose showed the presence of seven cross peaks of anomeric protons and carbons at δ (6.17 x 90.0), δ (5.68 x 91.0), δ (5.40 x 91.5), δ (5.37 x 91.5), δ (4.74 x 95.0), δ (4.6 x 101.0), δ (4.53 x 102.0), suggested that compound Eutheriose may be a hexasaccharide in its reducing form. The presence of seven anomeric proton and carbon were confirmed by seven anomeric signals of proton and carbon in the ^{1}H and ^{13}C-NMR spectrum of acetylated Eutheriose. The comparision of ^{1}H and 13C NMR of Eutheriose and it acetate confirmed the sequence of monosaccharides in it and position of glycosidic linkages which were confirmed by COSY, TOCSY, HSQC and HMBC and mass spectrometry. The structure of the novel oligosaccharide **Eutheriose** was confirmed as-

Compound Eutheriose- **α-GalNAc(1→4) α-Gal(1→3) β-GlcNAc(1→3) β-Gal(1→4) β-Glc**
|(1→2)
β-Gal

Key words- Eutheriose, oligosaccharide, buffalo milk

P-163

Synthesis of Benzofuran-dihydropyrimidinone hybrids and their biological evaluation as anti-Alzheimer agent

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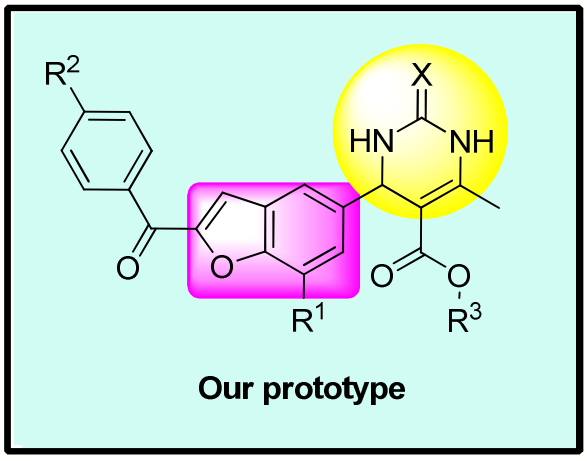
Alzheimer's disease (AD) is complex multifaceted progressive neurodegenerative brain disorder that affects millions worldwide.[1] There is an urgent need for additional research into more effective therapeutic options for the treatment of leishmaniasis. A series of hybrids bearing benzofuran and Biginelli adducts were synthesized as benzofuran derivatives has been explored and found to be effective against AChE and AChE-induced Aβ aggregation.[2] In addition, literature survey revealed that dihydropyrimidone and its derivatives are largely associated with cholinesterases.[3] The objective of this work was to investigate the anti-Alzheimer activity of these novel hybrids. Biological screening of synthesized compounds was undertaken in transgenic *Caenorhabditis elegens* model that expresses the human Amyloid *β* peptide. From a series of 20 compounds, compound **4f** and **4g** showed pronounced anti-Alzheimer activity. Effects of **4f** and **4g** on oxidative stress, paralysis, Aβ accumulation, and lifespan in the nematode *Caenorhabditis elegans* has been assessed.



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P-164

USE OF HETEROGENEOUS CATALYST TITANIA-SILVER (TIO_2-Ag) NANOCOMPOSITE IN SYNTHESIS OF DISUBSTITUTED QUINOLINES

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Heterocyclic compounds have a special role in organic chemistry because of their diverse biological properties. Among nitrogen-containing heterocycles, quinolines have high chemical and pharmacological significance and known to exhibit various activities such as anti-tumoral, anti-bacterial, anti-fungal, anti-malarial, and anti-inflammatory properties. Recently, the environmentally benign organic reactions and economically feasible catalysts are in high demand by chemical industries and considerable research effort is directed towards bottom-up synthesis of composite nanomaterials which combine the properties of two or more materials in a single product. Numerous reports describe the synthesis of such composite materials, with particular emphasis on immobilization of noble metal nanoparticles on oxides. Titania (TiO_2) is of interest due to their ready availability, ease of handling, low toxicity and low cost. It also offers favourable mechanical strength, thermal stability, high surface area, and very importantly allow adsorption of various solids and organic materials on their surface.

In continuation of our research programme toward the synthesis of biologically active heterocycles, we have developed a new protocol for syntheses disubstituted quinolines by three multicomponent reaction of arylamines, arylaldehydes and aliphatic aldehydes on surface of titania-silver (TiO_2-Ag) nonocomposite in excellent yields and very short reaction times for the first time. TiO_2-Ag nonocomposite was synthesized by wet chemical method.

The details of present work and mechanism will be discussed during the conference.

P-165

Sustainability As Benign Solution For Future

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ABSTRACT: Sustainability gives the idea for policies and strategies that meet society's present economic, social and environmental needs without compromising the ability of future generations to meet their own needs and chemistry is open the scope to finding sustainable solutions to far-reaching challenges, including: Energy provision, Environmental protection, Food and water safety, Global healthcare.

Innovations are investigated exemplarily for a sustainable development with regard to their ecological, economical, and social dimensions from an integrated and interdisciplinary perspective. Since base chemicals are produced in large quantities and important product lines are synthesized from them, their resource-saving production is especially important for a sustainable development. In the long run, renewable resources that are catalytically processed could replace fossil raw materials. Separation methods existing today must be improved considerably to lower material and energy consumption. Chemistry might become the pioneer of an innovative energy technique. The design of chemical products should make possible a sustainable processing and recycling and should prevent their bioaccumulation. Methods and criteria to assess their contribution to a sustainable development are necessary.

Key Words: Sustainability, bioaccumulation

P-166

WATER MEDIATED SYNTHESIS OF FUSED PYRIMIDOPYRIDINES USING WATER STABLE AND EFFICIENT CATALYST UNDER SONICATION

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Fused pyridine derivatives are an important family of organic compounds because they have broad range of biological and pharmacological activities. Thus, the synthesis of such compounds has attracted considerable attention of chemists. Recently, in modern society, more focus of researchers is based on synthesis of industrial and pharmaceutical important compounds using green innovative methods. In this regard along with various factors, solvents and catalysts play an important role because they represent a new way to meet the challenges of energy and sustainability. According to Sheldon "best solvent is no solvent and if a solvent needed it should preferably be water". Water is cheap, safe and eco-friendly solvent and reactions in water demonstrate unique reactivity and selectivity than other solvents. In continuation of our endeavor toward environmentally benign synthesis of biologically active heterocycles, herein we report a water mediated highly efficient and domino synthesis of fused pyrimidopyridines by the one pot condensation of 6-amino-1,3-dimethyluracil, aldehydes and cycloketones using Lewis acid surfactant combined catalyst under sonication. Lewis acid surfactant combined catalyst is a new catalyst acts as dual role both as a catalyst and surfactant. The simple experimental procedure, high yield, recovery and reusability make this protocol attractive. The mechanistic path of this reaction involves first formation of imine derivatives and their conversion to desired product by (4+2) cycloaddition reaction.
The details of present work and mechanism will be discussed during the conference.

P-167

Temperature dependent Raman studies of free standing thin films of Cellulose

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Abstract: Cellulose is an organic compound consisting of several linked D-glucose unit (Figure 1). Cellulose occurs naturally and is hence environment friendly and bio degradable. Using cellulose as semiconductors is cost effective and also does not pollute the environment. In this paper we study the low temperature vibrational properties of cellulose to understand about its bond characteristics at low temperature to widen the range of applicability of cellulose based semiconductors.

Free standing thin films of Cellulose were prepared by sol-gel method from extracts of banana plant. Raman spectroscopy was performed using Renishaw Invia Raman spectrometer using 785nm diode laser operating at 1% of its maximum power. The temperature was varied from -193^{0}C (LN_2) to room temperature using a Linkam Holder.

The Raman spectra for Cellulose at few different temperatures are shown in figure 1. Major peaks are observed at ~381cm^{-1} [1] , ~437 cm^{-1} ,~518 cm^{-1} , ~1096 cm^{-1} , ~1120 cm^{-1}, ~1460 cm^{-1} , ~2893 cm^{-1} and ~4094 cm^{-}1 which are characteristic of cellulose representing the various modes of C-, H -and O-bonding [2].

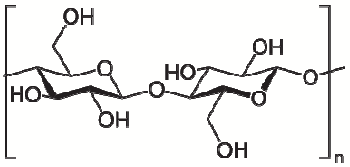

Figure 1: Cellulose structure

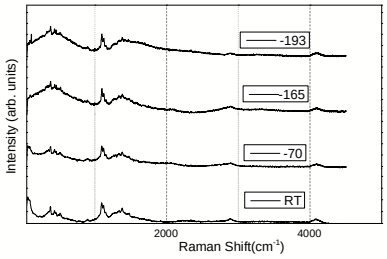

Figure 2: Raman spectra of cellulose thin film at different temperatures

With lowering temperature the 1460 cm^{-1} peak diminishes corresponding to H-C-H and H-C-O bending, indicating change in bonding environment. Again with lowering temperature many shoulder peaks appear very close to each other in the range 1100cm^{-1} to 1500cm^{-1}.

Keywords: Raman studies, Cellulose, Polymer Semiconductors

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P-168

Molecularly imprinted polymer-basedelectrochemical sensor for the ultra-trace electrochemical analysis of Cyanocobalamin in real samples.

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ABSTRACT: A novel methyl blue adsorbed rGO and f-MWCNTs composite functionalized with acryloyl urea was prepared which served as a dendritic monomer for the synthesisof Cyanocobalamin (Cbl) imprintedpolymer. A molecularly imprinted polymer based electrochemical sensor has been fabricated on the surface of pencil graphite electrode (PGE) for the analysis of Cbl. Graphene-CNT hybrid nanomaterials exhibit higher electrical conductivities, larger specific surface area, and better catalytic properties compared with either pristine CNTs or graphene (Kong et al.)[1] (Saleh et al.) [2]. Perpendicular assembly of rGO sheet and functionalized MWCNTs provide enhanced kinetics and conductivity to the polymeric films. This architectural designing in MIP film enhances the sensitivity of electrode.Cyclic voltammetry and differential pulse anodic stripping voltammetry has been employed for ultra-trace detection of Cbl. The calibration graphs plotted with differentconcentrations of Cblwas linear with a regression coefficient R^2> 0.9997. The detection limits realized by the proposed sensor, under optimized analytical conditions, were found to be as low as 0.01ng mL^{-1}Cbl(S/N = *3*) in aqueous, biological and pharmaceutical samples.Result showed that the modified PGE was highly simple, fast, cost effective, and feasible for the electro-analytical determination of Cblin real samples.

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P-169

Low Temperature Raman Studies of freestanding and flexible thin films of CdS doped PVDF

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Abstract:

PVDF(Polyvinyldene fluoride) is an organic polymeric compound having chemical formula $(-C_2H_2F_2-)_n$. It has been widely studied for its semiconducting properties. It usually exists in the □□ and the □□□ phases, with the □□□□□□□□□showing□ very good piezoelectric properties which enhances its use in modern electronic devices. In this paper we report the temperature dependence vibrational properties of PVDF/CdS to widen its arena of applications in low temperature regimes.

Free standing thin films of PVDF with nanocrystalline CdS were prepared by sol-gel method. The films were studied for vibrational spectroscopic properties using a Renishaw InVia micro Raman spectrometer . A 785nm diode laser was used for characterization operating at 1% of its operating capacity. To study the temperature dependence of the spectra the temperature of study was varied from room temperature to LN_2 temperature using a Linkam holder.

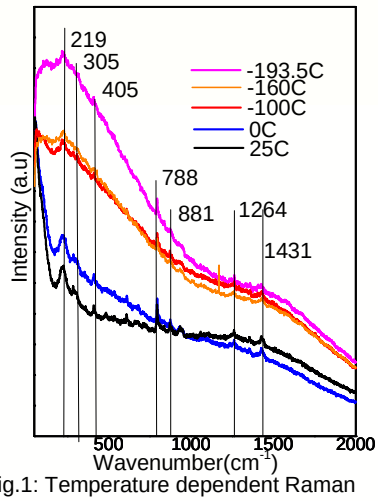

Fig.1: Temperature dependent Raman spectra for CdS/PVDF thin films

Figure1 shows the Raman spectra for PVDF/CdS sample at a few different temperatures. Major peaks observed at ~534 cm^{-1}, ~795 cm^{-1} and ~ 873 cm^{-1} corresponds to different vibrational modes of PVDF[1]. For CdS two major peaks ~295 cm^{-1} and 305 cm^{-1} were observed [2].

Intensities of the peaks seemed to decrease with decrease in temperature suggesting possible freezing of modes. Suppression of the peak at 881 cm^{-1} signifies the absence of some of the phases or conversion of one phase to another in the material [3].

Keywords: PVDF, polymer semiconductor, LT Raman

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P-170

BIOCIDAL ACTIVITIES OF DE-NOVO MIXED LIGAND SCHIFF BASE COMPLEXES OF TRANSITION METALS

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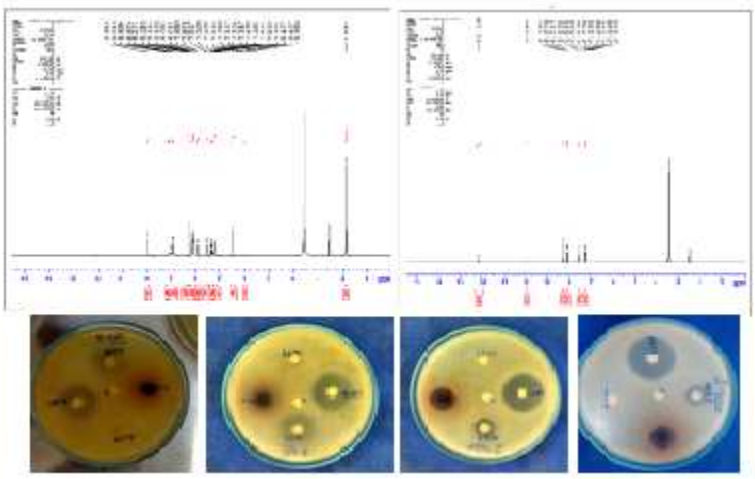
Abstract: Schiff's base compounds containing azomethine linkage formed by the condensation of carbonyl compounds to various amino compounds have been widely synthesised and characterised for decades. Of course, the thriving force behind the current researches in this field is due to its wide range of applications owing to their catalytic activity, photo fluorescent properties, use in dye industry *etc*., also due to their prodigious use in the pharmacological field as antibacterial, antifungal, anti-malarial, antitubercular and anticancer drugs. The DNA binding and cleavage studies of the metal complexes of Schiff's base containing heterocyclic moieties also have received much attention in recent researches in this field.The present work deals with the synthesis and characterization of a new series of Mn(II), Co(II), Ni(II), Cu(II) andZn(II)mixed ligand Schiff base complexes derived from indole-3-carboxaldehydewith 4-aminopyridine and 1,10- phenanthroline.Both the ligand and the mixed ligand complexes were characterised by elemental analysis, FT-IR,^{1}H NMR and UV-Vis. spectral studies.The magnetic measurements and also conductance studies of complexes were carried out in various solvents. The surface topography of the prepared compounds were studied by taking SEM. Single crystal XRD of the prepared copper complex was also taken for structural study. Both the ligand and the complexes werescreened for antibacterial activity against the bacterial species, *S. Aureas,E. coli* and for antifungal activity against *A. Niger*by disc diffusion method.



P-171

Efficient Method for Regioselective Vicinal Iodofuntionalized molecule by using Sulfonium Iodate(I) Reagent

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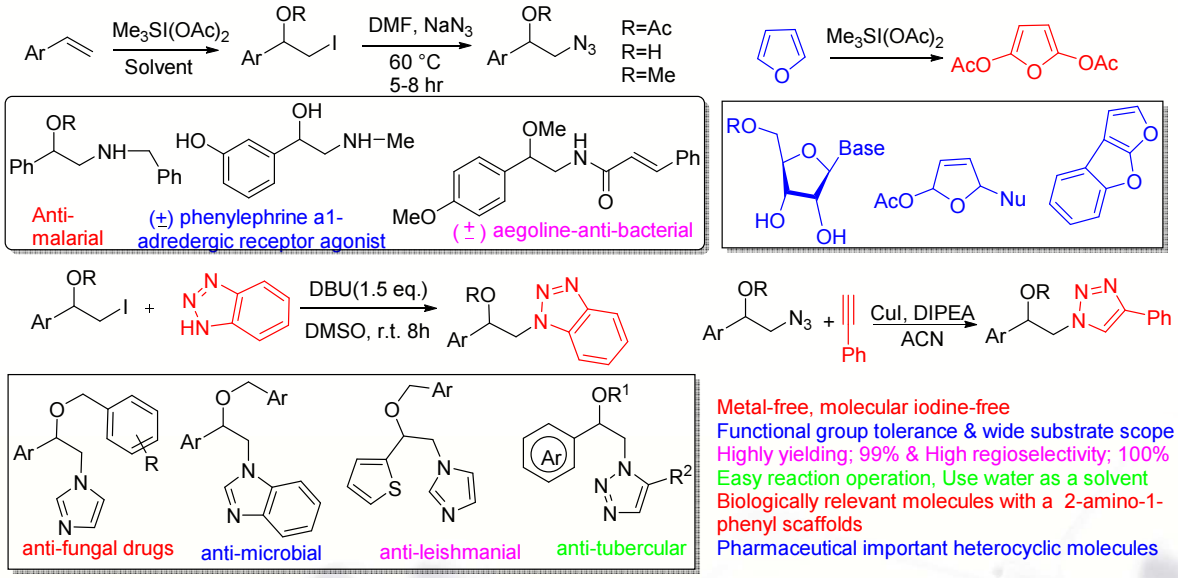
The stereoselective and regioselective disfunctionalization of olefins has been recognized as an useful transformation to pharmaceutically valuable molecules and active natural products[1]. Particularly, halofunctionalization, also known as "cohalogenation" of alkenes, is widely studied and elegant reaction enabled selective and facile addition of two new chemical entities in single step[2]. We recently demonstrated the preparation of novel sulfonium bis(acetoxy)iodate(I) reagent and studied its utility in iodoglycosylation of glycals. The exceptional versatility of metal-free protocol highlighted for one-pot and divergent synthesis of glycosyl carboxylates and glycosyl azides in stereo- and regioselective manner.[3]

The efficiency and convenience of present reagent system encourage us to relate this method mechanistically for bisfunctionalization of unactivated C=C double bond. This method enables the divergent and straightforward preparation of synthetically useful functionalities; β-iodocarboxylates, β-iodohydrins, and β-iodoethers in a one-step process. Further interconversion of iodo-functionalized derivatives allows easy access to valuable synthetic intermediates en route to biologically active molecules.



Stereodivergent bisfunctionalization of alkenes and Access to Important Scaffolds

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P-172

Analysis of chemical constituents of *Oldenlandiaumbellata* using LC-MS

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Abstract- *Oldenlandiaumbellata* belonging to Rubiaceae family has been reported to treat asthma, bronchitis, tuberculosis and inflammation. Investigating the chemical constituents of a bioactive extract is quiet essential to validate its pharmacological effects[1]. Taking note of this, analysis of chemical constituents of *O. umbellata*using LC-PDA-ESI-MSmethod was undertaken.

*O. umbellata*was extracted using methanol and the methanolic extract was suspended in water and subjected to solvent-solvent partition using ether and n-butanol to obtain OUEF and OUBF, respectively. Analysis of OUEF and OUBF were carried out using Shimadzu LCMS-2020 single quadrupole equipped with electrospray ionization (ESI) interface. HPLC was performed on LC20AD liquid chromatography, using Shim-pack XR-ODS column. The mobile phase consisted of pump A(0.4% v/v HCOOH in MilliQ water) and pump B (MeCN) following gradient elution technique with a flow rate of 0.3 mL/min.

While OUEF demonstrated presence of eighteensmall molecules, OUBF showed ninesmall moleculesi.e. having molecular weight <500. The identified compounds of OUEFwere 1,2-dimethoxy anthraquinone, hedyotiscone, 1,3-dimethoxy-2-hydroxy-anthroquinone, 1,2-dimethoxy-3-hydroxy-anthroquinone, 1,2-dimethoxy-3-hydroxy-anthroquinone acetate, 1,2,3-trimethoxy anthroquinone, ursolic acid, oledicoumarin, pheophorbide A-methyl ester. Further, OUBF was found to possessscandoside, 6α-hydroxygeniposide, feretoside, asperulosidic acid and deacetylasperuloside.

In conclusion, *O. umbellata* was identified to yield secondary metabolites like coumarins, anthroquinones, iridoidsandirodoid glycoside derivatives as major constituents.

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P-173

DENSITY FUNCTIONAL THEORY, BIOLOGICAL ACTIVITIES AND COORDINATION MODES OF COBALT(II) AND NICKEL(II) COMPLEXES OF SCHIFF BASE DERIVED COUMARIN LIGANDS

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Abstract: Coumarin derivatives exhibit broader applications in the field of pharmacological and biochemical properties. In the present study, the bioactive coumarin derivative and its cobalt(II) and nickel(II) complexes were synthesized. They were subjected to different analytical and spectroscopic techniques like FT-IR, ^{1}H and ^{13}C-NMR, mass spectroscopy, TGA, elemental analysis, molar conductivity and magnetic moment techniques. Nanocrystalline and morphological features of ligand and its complexes were investigated by powder XRD and SEM analysis. DFT studies of ligand and its complexes have been carried out using DFT-B3LYP/6-311++G(d,p) level of basis set. The calculated HOMO- LUMO energy gap values reveal that the charge transfer occurring within the molecule. The synthesized compounds were screened for their antimicrobial activity against different bacterial and fungal strains. The interaction of these complexes with CT-DNA was performed using several spectroscopy protocols, which indicates that complexes bind to CT-DNA through intercalation binding mode. Moreover, DNA cleavage experiment was revealed that the complexes exhibited remarkable DNA cleavage activities in the presence of H_2O_2 *via* the generation of hydroxyl radical. The synthesized compounds may be used as artificial nucleases and anticancer drugs.

P-174

Kinetic studies ofepoxidationof alkene by *Musa paradisiaca*

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Abstract: The versatility of the epoxide is attributed to the oxirane function that can be opened by various nucleophiles or undergo elimination, reduction or rearrangementsto a multitude of more elaborate intermediates with the retention or inversion of chirality.[1-3] Therefore the development of efficient syntheticmethods for enantiomeric pure epoxides has been of fundamental research interest in both organic synthesis and biocatalysis.

Enzyme is a potent epoxidation biocatalyst that displays moderate to high enantioselectivity on a wide variety of olefinic substrates[4-8].This communication reports a crude preparation of enzyme from plantwhich can be conveniently prepared and used for the transformation of alkeneto its epoxide.This is the report of epoxide formation using a plant enzyme.

The method for the preparation of enzyme from the plant has been developed. The steady state kinetics parameters, Km and $k_{cat}$of the enzyme for the indene, styrene, 4-chlorostyrene, 3-chlorostyrene, 2-chlorostyrene,4-bromostyrene and naphthalene have been determined in the presence of H_2O_2 and t-butyl peroxide as oxidants. The results of the above studies will be presented in the conference.

Key words: Enzyme, epoxide, alkene, *Musa paradisiaca*.

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P-175

Synthesis of new organophosphorus pesticides: phosphorylated Schiff bases of salicylaldehyde

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Abstract: Organophosphorus compounds are one of the most important group of modern pesticides [1-4]due to their high insecticidal and acaricidal activity, the broad spectrum and rapidity of action on pests. Various types of organophosphorus compounds have been synthesized and their biological activities have been tested. However literature survey has indicated that phosphorylated Schiff bases of salicylaldehyde have not been synthesized and their biological activities have not been tested. In this communication the synthesis and spectral characterization of diethyl 2- (phenyl imino) methyl phenyl phosphate and 2-(4-chlorophenylimino) methyl phenyl diethyl phosphate will be presented.

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P-176

Synthesis and bio-evaluation of indole-chalcone based benzopyrans as promising antiligase and antiproliferative agents

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DNA replication and repair are complex processes accomplished by the concerted action of a network of enzymes and proteins. DNA ligases play a crucial role in these processes by catalyzing the nick joining between DNA strands [1,2,3]. As compared to normal cells, elevated levels of human DNA ligase I (hLigI) have been reported in some cancers. We studied the inhibition of hLigI mediated DNA nick sealing activity followed by the antiproliferative activity of novel indole-chalcone based benzopyran compounds on cancer cells. One compound showed a notable preference for inhibition of hLigI as compared to other ligases and showed enhanced cytotoxicity against colon cancer (DLD-1) cells as compared to normal cells. This novel and potent hLigI inhibitor showed significant inhibition of both monolayer cultures as well as 3D culture of DLD-1 cells that mimic solid tumor. This novel hLigI inhibitor could therefore serve as a promising lead for anticancer drug development.

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P-177

ECO FRIENDLY TECHNIQUES FOR SURFACE MODIFICATION OF TEXTILE POLYMERS: A REVIEW

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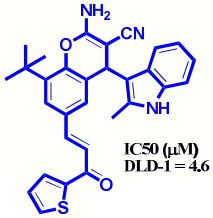

active compound

Abstract: Eco-friendly processing and techniques are gaining popularity nowadays for surface modification of textile polymers because of health hazards associated with the use of conventional methods.Textile polymers are used in a variety of applications which include clothing, carpeting and furnishing etc. In all these applications, surface modification is of profound importance as it improves various properties such as softness, roughness, crystallinity, lubricity, dyeability, absorbance and wettability [1]. There are various methods available for surface modification which are broadly classified under Chemical, Physical, Biological and Mechanical techniques. In this review, Physical Methods namely Cold Plasma Treatment [2], Corona Discharge [3] and UV Radiationare considered as finest environmental-friendly methods.All three of them are essentially dry processes providing modification of the top nanometre surface leaving bulk properties of the material unaffected without using solvents or generating any chemical waste [4]. The treated polymer surface performs differently as a function of their chemical structure, type of exposure i.e. plasma, corona or UV and exposure time [5].

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P-178

SEQUESTRATION OF ANILINE FROM AQUEOUS SOLUTIONS USING ZEOLITIC MATERIAL ADAPTED FROM BAGASSE FLYASH

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Abstract: Aniline laden industrial effluents constitute pollution threat to man. For industries to maximize profit while taking environmental safety into consideration, there is need to apply cheap, yet effective methods for secluding aniline from industrial effluents prior to disposal into aquatic environment. This work presents the sequestration of aniline from aqueous solutions by a zeolitic material synthesized from bagasse flyash which is a waste material from a sugar industry and obtained at no cost. The zeolitic material was characterized with XRD and XRF. Batch experiments were conducted to study the effects of parameters: pH of aniline solution (3-10); initial concentration (25-200mg/L); adsorbent dosage (0.25-5.00g/L) and adsorbent-adsorbate equilibration time (15-180minutes). At dosage 2g/L and initial concentration 100mg/L, optimum pH was 6 with q_e25mg/g which is equivalent to 50% aniline uptake. Likewise, 2 hours was enough for equilibrium interaction between the adsorbent and aniline. Furthermore, q_e was found to increase with increasing initial concentration of aniline, whereas was found to decrease with increasing adsorbent dosage. The studied synthetic flyash zeolitic material significantly sequestrated aniline from aqueous solution and therefore may be considered a cheap adsorbent for treating aniline laden effluents.

Keywords: Pollution, aniline, sequestration, bagasse flyash, zeolitic material.

P-179

A Diatom Based Bio-inspired Nanomaterial for An Efficient Self-Propelled Motor System

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ABSTRACT: Bio-inspired nanomaterials are of great interest because of their compatibility and less toxicity to nature. Diatoms have been employed due to not only their unique structure, but also the robust skeleton comprising silica. Moreover, the presence of trace amounts of transition metals endows versatile catalytic activity for various conversions. In this work, we are going to present an innovative methodology to use naturally occurring diatom frustules as a self-propelled motor machine after pyrolysis via the bubble propulsion by catalytic decomposition of H_2O_2. In this process, the use of toxic chemicals was avoided, which allows green and eco-friendly methodology for the preparation nanomaterial. This natural motor shows an effective motion in the presence of very low concentration of H_2O_2 (0.8%) as a fuel. In addition, asymmetric pennate (bilaterally symmetrical) structure can allow a unidirectional motion for the motor. The composition analysis of the pyrolyzed diatoms revealed the presence of transition metal elements which can expedite the decomposition of H_2O_2 fuel. Interestingly, the unidirectional motion breaking was observed by treatment of EDTA (ethylenediaminetetraacetic acid) that can stop the movement by coordination to transition metal elements. The kinetics of the H_2O_2 decomposition process was determined by conventional titration proved that the decomposition process follows a pseudo first order kinetics. A systematic study of these elemental showed that the inherent transition metal element may play a crucial role in the fuel decomposition process. Details of this work will be presented.

Keywords: Diatom; Molecular machine; H_2O_2; Motion; Control; Kinetics

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An Efficient approach for Synthesis of Bioactive Pyrazole carboxamides and their anticancer and antifungal activities

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Abstract: Pyrazole carboxamides are important compounds in the past few decades because they have found to be extremely key intermediates for the preparation of new biological materials. The pyrazole ring is present in area of medicines[1] and agrichemicals.[2] Amide functionality is one of the most fundamental chemical building blocks found in nature. It constitutes the backbone of the biologically crucial proteins, and it is present in a vast number of synthetic structures. Peptides and protein play a wide variety of roles inliving organisms and display a range of properties, from the potent hormonal activity of some smallpeptides to the structural support and protection for the organisms shown by insoluble proteins. In an industrial context, formation of the amide bonds represents the single largest subject in all reactions conducted in medicinal chemistry laboratories. A key step is the formation of the peptide bond, which involves amide bond formation. This requires the activation of a carboxylic acid, which is usually carried out by using peptide coupling reagent. Amide bonds are generally synthesized from the reaction of carboxylic acids and amines. Amide bond is essential to sustain life, making up the peptide bonds inproteins, such as enzymes, and it is also one of the most prolific moieties inpharmaceutical molecules, agrochemicals and natural products. The synthetic strategy adopted was the coupling of appropriately substituted amine derivatives with carboxylic acid. Structures of newly synthesized compounds were confirmed by ^{1}H NMR, ^{13}C NMR and synthesized compounds have been screened for *in vitro* antifungal activity and anticancer activity against MCF-7 cell line. Some of the compounds showed significant activity.

Keywords: Pyrazole carboxamides, Amide bonds, spectral studies, antifungal, anticancer activity

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P-181

Utilization of algae as a constituent of sustainable phytoremediation and renewable biomass for liquid fuel

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Dwindling fossil fuel reserves in coming century might face the challenge to develop 'eco-friendly', efficient and sustainable resource of energy. To date vast studies have been done to find out the super species of algae for efficient production of biofuel. However, biotechnological and molecular approaches seems to failure at commercial level due to environmental induced fluctuation which significantly decreased the efficiency of laboratory made species and high cost.

The use of algae for the cleaning of polluted water (phytoremediation) is a cost effective strategy to derive additional benefits from such remediation activities. The biomass generated can be used as a low-cost substrate for producing valuable bioproducts such as biofuels, ethanol and biocompost. Naturally grown algae possessed genetically and evolutionary difference to each other beacuase of their growth conditions and habitat, thus, itself develops the untapped potential of lipid production and phytoremediation. In this way, we tried to find out the most biomass producing algae having high content of lipid. Further, algae used in the phytoremediaition may be a potent candidate for resource recovery of nitrogen and phosphorus present in waste water and reintroduced them in the nutrient cycle by mean of organic fertilizers. This study may provide a new insight in the field of algal based biofuel generation, identification of algal communities that naturally exhibit high biofuel potential and phytoremediaiton.

Keyword: Algae, Biofuel, Phytoremediation, Biocompost

P-182

SYNTHESIS, CHARACTERISATION AND BIOLOGICAL EVALUATION OF SOME NEW CHALCONES, AMINO PYRIMIDINES AND ISOXAZOLES DERIVATIVES INCORPOTATING 1,3,5-TRIAZINE MOIETY

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ABSTRACT: Literature survey reveals that chalcones and their derivatives show good biological activities such as analgesic, antiviral, antimalarial, antibacterial, antitubercular etc.. Hence, from literature survey and due to different biological activities of chalcones, the condensation reaction of 2 - (tetrahydro-1',4'- oxazine) - 4 - (aminoethyl) - 6 - [4'- acetylphenylamino] - s - triazine in the presence of alkali with various aromatic / heterocyclic aldehydes gives chalcones which on cyclization with guanidine hydrochloride and hydroxylamine hydrochloride in presence of alkali give amino pyrimidines and isoxazoles respectively. The characterization of synthesized compounds has been carried out on the basis of IR, ^{1}H NMR spectral data as well as elemental analysis. The newly synthesized derivatives were screened for their *in vitro* antimicrobial activities against two bacterial and two fungal strains.

KEYWORDS: Chalcones, Amino pyrimidines, Isoxazoles, Spectral data, Antimicrobial

P-183

The cholesterol aided micelle to vesicle transition of a cationic gemini surfactant (14-4-14) in aqueous medium

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Abstract: The cholesterol (Chol) induced micelle to vesicle transition of a cationic Gemini surfactant (tetramethylene-1,4- bis(dimethyltetradecylammoniumbromide; 14-4-14) has been investigated by using spectrophotometry (UV-visible and fluorescence), Dynamic Light Scattering (DLS), High Resolution Transmission Electron Microscopy (HRTEM), etc. at different R ([Chol]/[G.S]) values. The optical density gradually increased from R=0 to R=1 with increasing R value and it was highest at R=1. The absorbance and fluorescence spectra of R=0 to R=1 also showed that shifts of the absorbance and fluorescence spectra towards the blue region, which supported transfer of micelles to vesicles. This was supported by the DLS measurements. The hydrodynamic diameter of the micelle was 0.84 nm whereas the vesicle diameters fell in the range of 160 nm -240 nm which is obtained from HRTEM measurements.The steady state fluorescence anisotropy using hydrophobic membrane bound probe 1,6-diphenyl-1,3,5-hexatriene (DPH), was also studied which shows increase in the restriction of probe motion with the addition of cholesterol. Structural incongruence of the mixtures changed the anisotropy values. The rotational relaxation time of C153 (Coumarin 153) was studied from time resolved fluorescence anisotropy. With increased R values the rotational relaxation time increased. The probe molecules found more rigid environment and its rotation time increased compared to the normal environment.

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Metal-Free, Phosphonium Salt-Mediated Sulfoximination of Azine N-Oxides: Approach for the Synthesis of N-Azine Sulfoximines

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Abstract: Herein, we report a simple and metal-free method for the synthesis of *N*-azine sulfoximines by the nucleophilic substitution of azine *N*-oxides with *NH*-sulfoximines. The present method works at room temperature with wide functional group compatibility and gives several unprecedented *N*-azine sulfoximines. The reaction conditions were also found suitable with enantiopure substrates and furnished products without any racemization. It also finds an application in the sulfoximination of azine-based functional molecules such as 2,2′-bipyridine, 1,10-phenanthroline, and quinine.

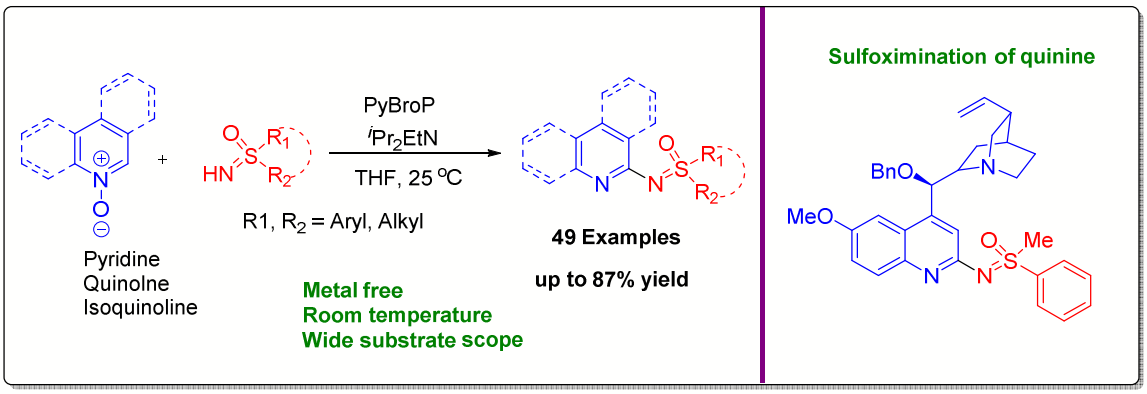

Figure: Studies toward the Synthesis of *N*-Azine Sulfoximines

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MEDICINAL CHEMISTRY ON NITROIMIDAZOOXAZOLINES: TRIAZOLYL CONTAINING 6-NITRO-2, 3-DIHYDROIMIDAZOOXAZOLE COMPOUNDS AS NEWER GENERATION ANTI-TB AGENTS

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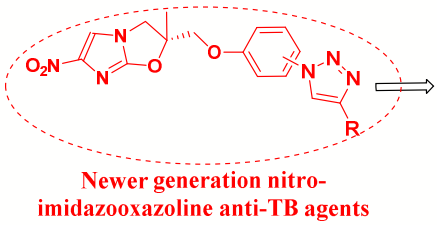
Tuberculosis (TB) remains a leading infectious disease worldwide and infected about one-third of the world's population. World Health Organization (WHO) reported that TB caused more than 10.4 million cases of illness and 1.5 million deaths globally in 2015.[1] Emergence of multidrug resistant TB (MDR-TB) and extensively drug resistant (XDR-TB) has further complicated the world situation.[2] Therefore, the current situation necessitates the discovery and development of new anti-tuberculosis agents with low toxicity profiles and having potency against both drug-susceptible and drug-resistant MTB. In the last decade, nitroimidazole skelton developed great interest among the researchers of academic and industrial fields, which lead to the discovery of two anti-TB clinical candidates namely PA-824 and OPC-67683. In this direction, we have initiated a medicinal chemistry programme on nitro-imidazolooxazoline skelton to generate a newer generation anti-TB agents. Small focused library of triazolyl containing 6-nitro-2, 3-dihydroimidazooxazoles derivates generated, lead to the identification of new lead molecule **IIIM-AF-01** which has shown potent minimum inhibitory concentration (MIC) of 0.06 µg/ml against sensitive and resistance strains of MTB and also active against non-replicating strain of MTB 18b. **IIIM-AF-01** has improved solubility, safety profile as well as excellent oral pharmacokinetic profile with 59% oral bio-availability.



IIIM-AF-01 ⟹

MIC H_{37}Rv MTB	= 0.06µg/ml
MIC Rif^RMTB	= 0.05µg/ml
MIC MDR MTB	= 0.5 µg/ml
NRP	= 2 µg/ml
PK @ 5mg/kg P.O	
C_{max}	= 0.943 µg/ml
AUC_{0-t}	= 7.6 µg/ml*h
Oral bioavailability(F%)	= 59%

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Blue to Green color tunability of rare-earth trivalent doped ion in BLZO nanophosphor

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Abstract: Aseries of trivalent terbiumdoped BLZOnanophosphors with concentration from 0.5 mol % to 3.5 mol % was synthesized via ureaassisted solution combustion method using metal nitrates as initial resources.The Rietveld analysis exhibited that these nanophosphors grow in the tetrahedral phase with the 14*/mcm* (140) space group.The surface morphology and photo-luminescent properties of the sample were examined by TEM, PXRD and photoluminescence (PL) spectra long with fluorescence life-time decay profile. The particle diameter was assessed by Scherrer's equation and TEM micrograph which was found in good agreement results as 65nm (approximate crystallite size). The photoluminescent excitation of these nanocrystals study ofBLZO: Tb^{3+}exposed that the excitation at 272 nm yields the characteristic emission peak at 545 nm ($^5D_4 \rightarrow {}^7F_5$)responsible for green color (at high concentrations) and 413 nm ($^5D_3 \rightarrow {}^7F_5$) responsible for blue color (at low concentrations) as cross-relaxation and quadrupole- quadrupole transitions of Tb^{3+}ions. The commendable luminescent contour of these nano-scaled particles proposes their fortunate applications in the solid-state lighting and display technology.

Keywords: Solution-Combustion, Photoluminescence, Nanophosphor, Color-tunable, Crystal structure, Energy transfer,Photoluminescence

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Metal catalyzed room temperature oxidative acylation of heterocyclic *N*-oxide with alkynes

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Abstract: Herein, we report a simple and metal-catalyzed method for the synthesis of acylation by the nucleophilic substitution of *N*-oxides with alkynes. The present method works at room temperature with wide functional group compatibility and gives several unprecedented alkynes. The reaction conditions were also found to be suitable for late stage functionalization with Quinine, 2,2-Bipyridyl, 1,10-Phenanthroline and furnished products in good to moderate yield withregioselectivity.

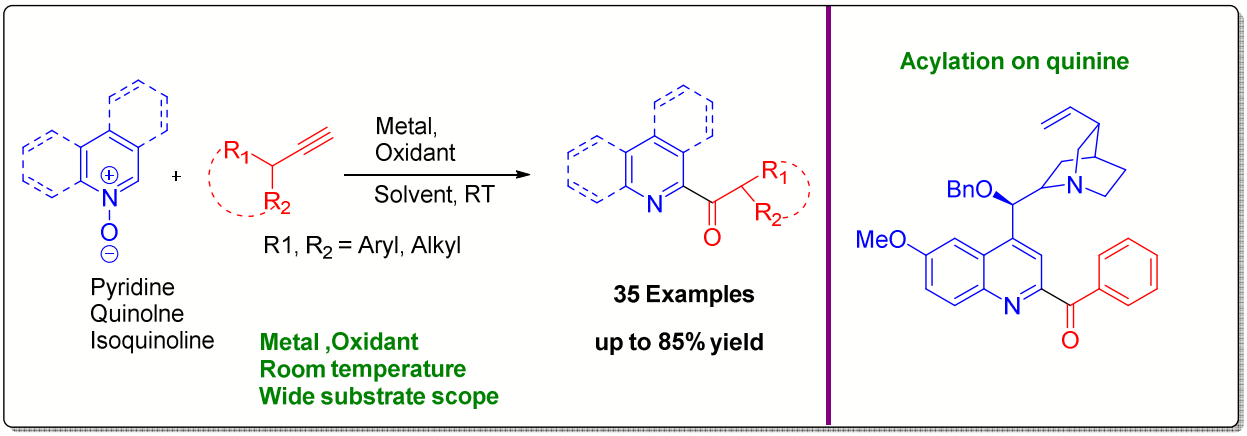

Figure: Studies toward the synthesis of classical Minisci Reaction

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Synbiotic preparation with Lactic acid bacteria and oligofructose enriched inulin as a functional food: *in vivo* evaluation of microbial activities and colorectal cancer

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Researchers suggested that the prevention of colon cancer might occur through intervention of synbiotics (prebiotic+probiotic) that allow certain substantial changes in the gut micro biota. The pro and prebiotic supplementation helps to improve the host health. Inulin is one such prebiotic used for the enhancement of naïve probiotic bacterial population. This paper explains the impact of inulin (PRE) extracted from taproots of common chicory (*Cichorium intybus L.*), *Lactobacillus salivarius* (*L. salivarius*) *FP25*, (PRO), and synbiotic (SYN; inulin + *L. salivarius FP25*) preparation on Azoxymethane mediated CC induced rat model with respect to changes in microbial load, microbial enzymes. The results suggested that the PRE and SYN supplementation effectively reduced the selected pathogenic bacteria (*Salmonella* spp., and *Escherichia coli*), microbial enzymes and increased the probiotic load. The intervention of SYN significantly reduced the colonic ACF in CC model. The study results revealed that the supplementation of SYN diet (inulin and *L. salivarius FP25*) protects the AOM-mediated colorectal cancer induced host.

Keywords: inulin; *L. plantarum*; probiotic; prebiotic; synbiotic, Chicory

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P-189

Targeting the Pyocyanin,Phenazine and quinolone: A paradigm for Combat with Persistantbehavior

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ABSTRACT: Intracellular chemical conversation process which ultimately expresses the group beneficial phenotype known as quorum sensing (QS).[1,2]*Pseudomonas aeruginosa*is gram negative bacterium, primarily infects immunocompromised individuals. In cystic fibrosis (CF), patients are susceptible to chronic lung infections. The most common bacteria cultured from CF patients is *P. aeruginosa*.[3,4] The pathogenicity is strongly related to the expression of large number of virulence factors which causes tissue damage, delay airway epithelium wound repair, and suppress innate immune response.[5]Targeting the main three networking systems *viz.* Las, RhI and PQS *via* natural quenchers is a new ray of hope for combating thepersistentbehavior of*Pseudomonas aeruginosa*. In the bacterial chemical vocabulary pyocyanin, N-AHLs and rhamnolipids are the main keywords, which are responsible for the social and nomadic behavior of *P. aeruginosa*. In the present work LCMS-based real time qualitative and quantitative analysis of pyocyanin, green phenazine, N-AHLs and rhamnolipids was performed. The quantitative analysis indicates that the production of pyocyanin and NHSLs increases with time while the production of Rhamnolipids discontinued after 24 Hrs. This indicates the emergence of persisters in the medium instead of planktonic cells. Rhamnolipids being acts as a surfactant enhances the motility of the bacterial cells, whereas, the pyocyanin is responsible for the biofilm formation. In microtiter plate based assay an effect of natural molecules was recorded. In the presence of natural molecule the production of rhamnolipids, phenazine , quinolone and N-AHLs was drasticaly decreases . Most interestingly, the IIIM-G treatment led to the decreases in rhamnolipids, phenazine , quinolone and N-AHLs. These studies demonstrates the effectiveness ofthe IIIM-G on Las, PQS and Rhl circuits in bacterium in order to understand the persistent and social behavior. Here we are reporting LC-MS based qualitative and quantitative analysis of QS molecules by taking a low volume of culture (up to 200 µl). This method can be used as a platform to screen the new antivirulence agents for fighting with resistant behaviour of *P. aeruginosa* during biofilm formation.

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Redox properties and cytoprotective activity of lichen substance from *lichen rangiferinus*

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Abstract :

Lichen rangiferinus, also known as reindeer lichen or caribou moss , is a light-colored, fruticose lichen belonging to the Cladoniaceae family [1]. It possess a variety of bioactive compounds including abietane, labdane, isopimarane, abietane diterpenoids hanagokenols A and B, ontuanhydride, sugiol, 7α-hydroxysandaracopimaric acid, 5,6-dehydrosugiol, montbretol, *cis*-communic acid, imbricatolic acid, junicedric acid, 15-acetylimbricatoloic acid, , , β-resorylic acid, atronol, barbatic acid, homosekikaic acid, didymic acid and condidymic acid [2]. Atranorin (ATR) and Fumarprotocetraric acid (FPA) are one of the major constituents of *Lichen Rangiferinus*. Here, we evaluated free radical scavenging activities and antioxidant potential of FPA using different in vitro assays for scavenging activity against hydroxyl radicals, superoxide radicals, hydrogen peroxide, and nitric oxide. The total reactive antioxidant potential (TRAP) and total antioxidant reactivity (TAR) indexes and in vitro lipoperoxidation were also evaluated. Besides, we determined the cytoprotective effect of FPA on H_2O_2-challenged HepG2 cells by the MTT assay. FPA exerted differential effects towards reactive species production, enhancing hydrogen peroxide and nitric oxide production and acting as a superoxide scavenger; no activity toward hydroxyl radical production/scavenging was observed. Redox analysis of FPA indicated that it also acts as a general antioxidant, though it was found to enhance peroxyl radical-induced lipoperoxidation in vitro. FPA was not cytotoxic, and also protected HepG2 cells against H_2O_2-induced cell viability impairment. Our results suggest that FPA has a relevant acting as a pro-oxidant or antioxidant agent depending on the radical. Also, it will exert cytoprotective effects on cells under oxidative stress induced by H_2O_2.

Keywords : *Lichen rangiferinus*, fumarprotocetraric acid, cytoprotective, antioxidant.

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CNT Reinforced Silver Nanocomposite: Effect of Sintering on their Electrical Conductivity

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Abstract: Silver/CNT nanocomposites have been fabricated using physical mixing method. Surface morphological studies have revealed that CNT's are uniformly distributed into silver matrix. Fabricated samples have been subjected to sintering for 12 hrs at 800^{o}C. Effect of sintering on electrical conductivity of the Ag/CNT samples is then analyzed. Electrical conductivity of both single wall carbon nanotube (SWCNT) and multiwall carbon nanotubes (MWCNT) reinforced silver nanocomposites increased appreciably upon sintering.

Keyword: Nanocomposites, Sintering, Electrical Conductivity, SWCNT, MWCNT

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β-Cyclodextrin Catalysed C-C Bond Formation *via* C(sp^3)-H Functionalization of 2-Methyl azaarenes with Diones in aqueous medium

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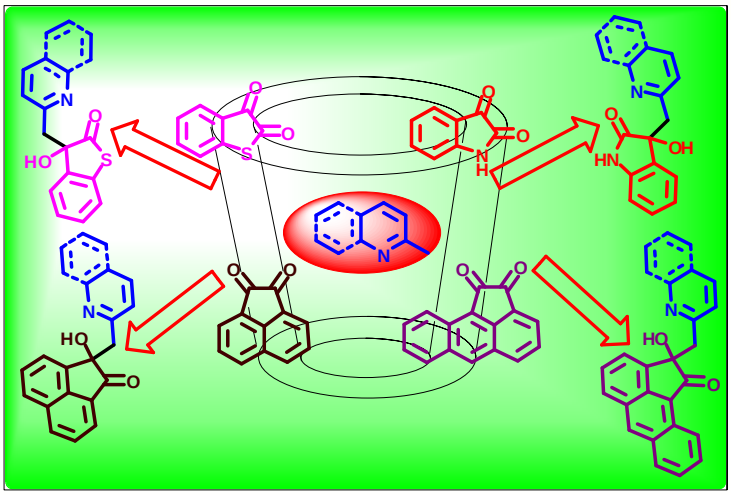
First β-cyclodextrin catalysed C(sp3)-H functionalization of 2-alkyl-azaarenes with homocyclic as well as heterocyclic diones in water has been developed. This bio- mimetic catalyst oriented methodology provides a sustainable and green protocol for C-H functionalization, the area mainly dominated by transition metals



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Deep Eutectic Solvent Induced Diastereoselective Synthesis of (Z)-4-(2-hydroxyprop-1-en-1-yl)-1H-benzo[b][1,5]diazepin-2(3H)-one, and 4-(2-hydroxyphenyl)-1H-benzo[b][1,5]diazepin-2(3H)-one Derivatives as Anticancer Agents

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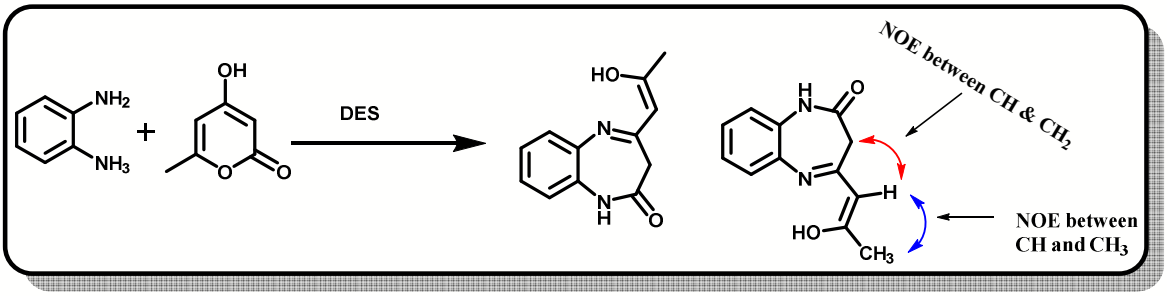
The first Deep eutectic solvents (Cholinechloride-Urea mixture) induced, efficient diastereoselective approach for the synthesis of (Z)-4 alkyl -1H-benzo[b][1,5]diazepin-2(3H)-one, and 4-aryl -1H-benzo[b][1,5]diazepin-2(3H)-one derivatives using o-phenylenediamines with 4-hydroxy-6-methyl-2H-pyran-2-one /4-hydroxy-2H-benzopyranone derivatives have been developed.The Deep eutectic solvents has reaction catalysing as well as designer medium capability, thus we named this strategy as Deep Eutectic Solvent Induced Reaction(DESIRE).



we have developed a practical and general protocol for the novel synthesis of (*Z*)-4-alkyl-1H-benzo[*b*][1,5]diazepin-2(3*H*)-one, and 4-aryl-1H-benzo[*b*][1,5]diazepin-2(3*H*)-one derivatives. This protocol offers significant improvements over many existing procedures with regard to yield of products, mildness of reaction conditions, simplicity in operation, selectively Z isomer, cost-efficiency, and above all, green aspects avoiding toxic catalysts and solvents.

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Synthesis of Annulated Dihydrofurans From Oxobis(methylthio)ketene Acetals and *N*-butyl-*N*'-methyl ethane-1,2-Diamine as Precursors Via NHC Elemination, Betaine Intermediate

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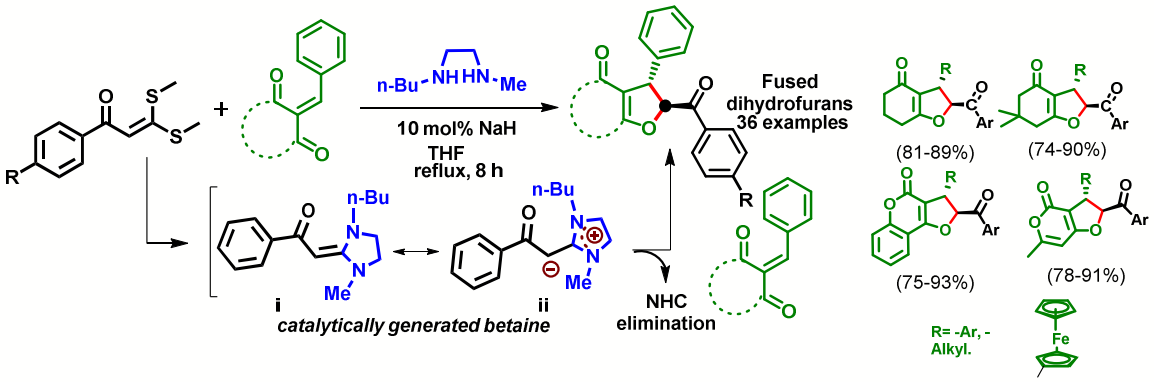
Abstract: First in-situ generation of betaine intermediate has been developed using two new precursors oxobis(methylthio)ketene acetals and N-butyl-N'-methyl ethane- 1,2-diamine for the synthesis of annulated dihydrofurans [1]. Our preliminary work has been based on organocatalysis as well as multicomponent reactions (MCRs) for the synthesis of various biologically important heterocyclic compounds [2,3]. In continuation this protocol adds a new dimension for the formation of annulated dihydrofurans through a series of selective consecutive formation of C-C & C-O bonds after reacting with enone rings. This in-situ generated betaine intermediate corresponds to deoxy-Breslow intermediate in the reaction via elimination of NHC.



Scheme: synthesis of annulated dihydrofurans via Betaine intermediate

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Polyphenolic acetate (7,8-diacetoxy-4-methylthiocoumarin) enhances proliferation of fibroblasts

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Polyphenols are naturally occurring anti-oxidants, studied widely for their mitigative effect on DNA damage by reactive oxygen species Venkateswaran et al. [1]. Studies on Polyphenolic Acetates (PAs) that can donate acetyl group and function like anti-oxidant are emerging A. Verma, et al. [2] 7,8-diacetoxy-4-methylthiocoumarin (DAMTC) is studied for its radiomitigative properties through epigenetic modulation. Recent study on DAMTC showed that when administered, whole body lethal dose irradiated mice had better survival rate by increased re-population in gastro-instestinal and haematopoetic systems Kavya et al. [3].

These evidences point towards a role of DAMTC as an enhancer of proliferation and a promising candidate for wound healing studies. Fibroblasts have a crucial role in wound healing; therefore the effect of DAMTC was tested *in-vitro* on human Adult Dermal Fibroblast (hADF) cell-line. The dosage standardisation was done by MTT assay and effective dose 5µM to 20 µM was used for subsequent studies. The proliferation rate of hADF was studied after exposure to 24 and 48 hours by Colony Forming Unit assay (CFU) and its effect on cell cycle was done by Propidium Iodide staining. Scratch wound assay was carried out to assess the effect on wound closure time and was visualized by live cell imaging microscopy. DAMTC was found to improve the wound closure versus time via enhanced proliferation of hADF. Further studies on *in-vivo* wound healing models will evaluate if DAMTC can be a cost effective additive to wound healing preparations.

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Tetra butyl ammonium cyanate mediated selective synthesis of sulfonyltriuret and their investigation towards trypsin protease modulation

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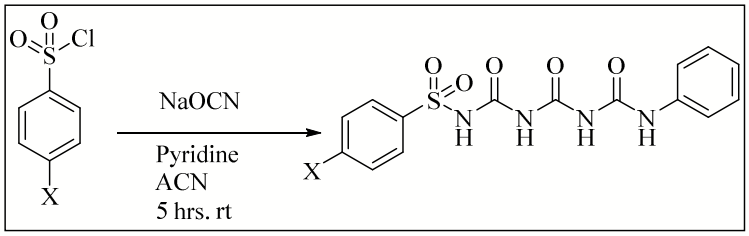
Pseudo peptide can mimic the biological or structural properties of natural peptides. They has become an increasing attention in medicinal chemistry because of their interesting advantages like more bioavailability and less biodegradation than compare to the physiologically active native peptides which increases their therapeutic applications [1].Many biologically active compounds contains urea as functional groups and they have improved pharmacokinetic properties because of their bioavailability and metabolic stability [2].Recently we have reported a single-step synthesis of sulfonyl urea and sulfonyltriuret from sulfonyl chloride and sodium cyanate [3] according to scheme 1. In the present work we mainly focused on the selective synthesis of sulfonyltriuret using tetrabutylammonium cyanate and sulfonyl chloride. The distinctive architecture of these molecules in the form of their pseudo-peptide backbone offers promise as a potential pharmacophore. The synthesized molecules have been screened on trypsin enzyme and we observed that these molecules are the efficient activator of trypsin enzyme.



Scheme 1. Synthesis of Sulfonylurea

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P-197

Controlled template free aggregation of dimeric carbocyanine dyes and its applications

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Self-assembled and programmable optical probes have ongoing attention in biomedical applications, especially in cancer treatement[1]. Cyanine dyes have long served as staining and imaging agents for biomolecules[2]. Cyanine dyes also undergo aggregation behaviour that is often unpredictable and creates challenges for their use. The template-directed aggregation of cyanine dyes has been comprehensively examined as a mechanism for formation of controlled dye aggregates. In this regard templates such as polymeric DNA duplexes and polyanions have been found to play a crucial role in controlling the aggregation of symmetrical dicarbocyanine dyes[3]. DNA-templated dye aggregation has highlighted the importance of dye-dimers as the building blocks of supramolecular assembly. Inspired by the DNA-templated assembly of cyanine dyes, we have developed and investigated the self-assembly of dimeric dicarbocyanine dyes. A series of N-linked dimeric benzothiazole containing trimethine and pentamethine cyanine dyes have been synthesised. Self-assembly of these dyes was confirmed with a variety of spectroscopic techniques. We observe a strong correlation between the length of linker connecting two dye units with their ability to preferentially dimerise and form extended aggregates. Aggregation propensity of trimethine dyes is distinctly different form monomeric trimethine dyes. The dimeric dyes are found to form H-dimers and H-aggregates without the need for external templates. In addition N-propyl linked pentmethine dimeric dye has aggressive self-aggregation behaviour in phosphate buffer solution in the micromolar range. Similar aggregates of the monomeric dicarbocyanine dyes are known to be observed at much higher dye concentrations or only in the presence of suitable templates. Pronounced aggregation of dimeric dyes raises the prospect of using fluorescence quenched H-dimers and H-aggregates as switch-on fluorescence probes in response to specific targets. The electronic structure of these dimeric dyes has been calculated and agrees with the observed optical spectroscopic behaviour. Further, we have studied the interaction of dimeric dye aggregates. Polymeric DNA templates such as $[poly(dA\text{-}dT)]_2$ leads to transformation of the spontaneously formed dimeric dye H-aggregates and H-dimers into DNA-bound dye species. Bovine serum albumin (BSA) exhibits a distinctive binding interaction with the dimeric dyes, unlike their monomeric counterparts. Implications of the dye self-assembly coupled with selective interaction with biomolecules are examined especially in the context of fluorescence signalling and imaging.

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P-198

Peptide enhanced Nanofiber scaffolds for Tissue Engineering

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3D scaffolds provide an optimalplatform allowing attachment, migration and organization of new cellular microenvironment Atala et al [1] thatinfluences stem cell fate and differentiation. Scaffold seeding is usually achieved by high cell density in minimal volumes to promote selective adherence. It also requires maintaining them so, for long durations to facilitate attachment. To counter this sub-optimal seeding process it would be advantageous to enhance them with strategies promoting adhesion in a shorter duration of time.

Lamininsplay an essential role in enhancing cell adhesion and focal assembly. Laminin α2 chain is specifically expressed in the basement membrane surrounding muscle and nerve Samuel et al [3]. Specific α2 mimicking peptides A2G51and A2G10Urushibata et al [4]were evaluated with muscle cell lines (unpublished data) for adhesion and MTT assay and a peptide concentration range of 0.1 to 1.0 µg was used for subsequent experiments.Isolated mesenchymal stem cells (MSCs) from Umbilical Cord tissue (n=4) after ethical approvalwereevaluated for their morphology and attachment versus time. The effect of the peptides on the MSCs was studied using propidium iodide staining and flow cytometry for cell cycle analysis. Phalloidin-TRITC staining was also carried out to analyze cell attachment and spreading by observing actin stress fibers and focal adhesion points.The A2G51 and A2G10 peptide coated nanofiber scaffolds exhibited more cell attachment versus time compared to the uncoated scaffolds and are promising candidatesfor applications in tissue engineering.

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P-199

A validated LC-MS/MS method for quantitative analysis of quercetinfrom *aeglemarmelos*in rat plasma and its application in pharmacokinetic studies

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Abstract

A simple and sensitive validated LC–MS/MS analytical method was used for determination of quercetin obtained from *aeglemarmelos* in rat plasma, using nimesulide as internal standard. Analyses were performed on an Agilent LC–MS/MS system using a Chromolith rod™ and isocratic elution with acetonitrile:10 mM ammonium acetate buffer (pH 3.5) (80:20, v/v) at a flow rate of 1.0 ml/min with a total run time of 5 min and an overall recovery of 75.16%[1,2]. A triple quadrupole mass spectrometer, equipped with an electrospray ionization interface, operated in the negative mode was used. Calibration curve in plasma spiked with varying concentration of quercetin were linear over the concentration range of 10–2000 ng/ml with determination coefficient >0.99. The lower limit of quantification was 10 ng/ml. Intra and inter-day variability's (RSD) for extraction of quercetin from plasma were less than 10% and 15% respectively and accuracy was 104.35–109.6%. Multiple reaction monitoring was used to monitor the transition for quercetin (*m*/*z*; 362/137 $[M-H]^-$). The method was applied for determining quercetin concentration in plasma after peroral administration of 50 mg/kg of free quercetin (Q-S) or quercetin loaded solid lipid nanoparticles (Q-SLNs) to rats. Results established selectivity and suitability of the method for pharmacokinetic studies of quercetin from Q-SLNs.

KeywordsQuercetin,LC–MS/MS, Liquid liquid extraction (LLE), Solid lipid nanoparticles (SLNs)

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P-200

Design, synthesis and anti-proliferative activity of small molecules as putative CDK4/6 inhibitors

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Cancer is multifactorial disease causeddue to uncontrolled cell cycle dysregulation that altersmitogenic signalling which is one of the important hallmarks of cancer [1-4]. The X-ray structures of cyclin dependent kinases (CDKs) and their structural insights are important aspects in the designing specific inhibitors[5]. Out of all CDKs, CDK4/6 has gained the importance as they have shown to play their role in driving cell cycle by phosphorylation of retinoblastoma protein. In the epoch of growing drug resistance, mutations and amplification of CDK 4/6, were observed in breast cancer patients[6-8]. The significant dysregulation of the CDK4/6-Rb phosphorylation has been reported by Finn et al; 2016 [9]. Palbociclibwas introduced into the market in 2015, while ribocicilib and abemacicilib are recently approved by FDA in 2017 as CDK4/6 inhibitors. The discovery of selective CDK inhibitors drugs has provided an effective strategy to treat cancer. In our work, we have designed, selective CDK4/6 inhibitors based upon imidazole nucleus and their synthesis and biological evaluation has been carried out as anti-cancer agents.

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P-201

Design, Synthesis and*In vitro* Evaluation of 3,5-Diaryl-4,5-dihydro-1*H*-pyrazole-1-carbaldehyde Derivatives: Potential for Xanthine Oxidase Inhibition in the Prevention and Treatment of Cancer

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Abstract: Xanthine oxidoreductases (XOR) isimplicated in the process of oncogenesis either directly because it is able to catalyze the metabolic activation of carcinogenic substances or indirectly through the action of XOR-derived reactive oxygen and nitrogen species[1]. Although multiple papers have been published that correlates XOR with cancer[2] but still there exist a high level of ambiguity on a crunch conclusion. In on our previous research[3-6] and current work based on the XO-febuxostat and topiroxostat interaction models we have thought of designing and synthesizing 3,5-diaryl-4,5-dihydro-1-carbaldehyde derivatives (**2**; Figure. 1) *via* structural modification of our reported non-purine series; *N*-(1,3-diaryl-3-oxopropyl)amides[7] (**4**) and *N*-acetyl pyrazolines (**5**)[8] with the following considerations: (i) favorable arene –arene interactions with Phe914 and Phe1009 with any one or two of the aryl/heteroaryl rings (mostly joined by three atoms); (ii) replacement of methyl group (-COCH_3) of **5** with hydrogen atom (-C*H*O of **2**) for one extra H-bond interaction with Glu 804 leading to better binding and; (iii) a site for hydroxylation near molybdenum metal.

The synthesized molecules were further evaluated *in vitro* for their xanthine oxidase inhibitory potential. The best screened compounds were taken further for their detailed anticancer activities that includes cell based assay, Western Blotting, RT-PCR, Cell cycle analysis, mode of cell death prediction, etc., The work has provided us the insights toward direct interaction between role of xanthine oxidase and cancer. The details and the important find outs will be discussed during the progression of conference.

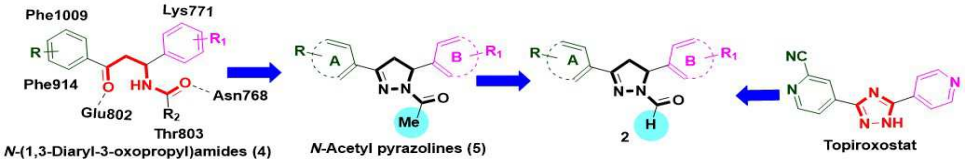

Figure 1: Design of target compounds (**2**) as xanthine oxidase inhibitors.

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P-202

Design, Synthesis, Molecular Docking studies of Novel *2-(4-(acridin-9-yl-amino)phenyl)isoindoline-1,3 dione* derivatives for their antibacterial and anticancer activities: A promising anticancer agents against Breast cancer

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Abstract: A series of 2-(4-(acridine-9ylamino)phenyl) isoindoline-1,3-dione derivatives **6a-6k** were synthesized in high yields and characterized by elemental and spectroscopic analysis. Among the synthesized, seven compounds **6a, 6b, 6e, 6g, 6h, 6i** and **6k** were evaluated for their antiproliferative activity against two human cancer cell lines, MCF-7 (breast cancer) and A-549 (lung cancer) by MTT assay. The results revealed that compound **6h** exhibited higher cytotoxicity againstMCF-7 and the compound **6i** against A-549 cancerous cell lines respectively. The docking studies were done for these derivatives against class I phosphoinositido 3-kinase (PI3K) isoform PI3Kα (5DXT) and MDM2 protein kinase by **Schrodinger Maestro 11.2 version**. The pthalimide substituted acridine derivatives **6a, 6b, 6e, 6g, 6h, 6i** and **6k** have significant anticancer activity as PI3Kα protein kinase for MCF-7 cancer cell line. More to the point the compounds were screened for their antibacterial activity, among these **6b, 6g** and **6h** exhibited excellent activity than the standard ***Ciprofloxacin*.**

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New Water Soluble N-heterocyclic Carbene Ruthenium(II) Complexes: Synthesis and Catalytic Application

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Water is a green solvent and an attractive alternative to volatile organic solvents in organic synthesis because water is non-toxic, non-volatile, non-flammable and inexpensive. In addition water is a renewable resources having high heat capacity which allow for safe handling of exothermic reactions. Recently N- heterocyclic carbene ligands have gained significant attention as supporting ligands for variety of metal catalysed reactions in water [1].Designing new water soluble N-heterocyclic carbene ligands and their metal complexes is an important area of research. Very few water soluble N-heterocyclic carbene ligands and their metal complexes have already been used in various organic transformations [2-4]. Towards this effort, we have synthesized 1,2,4-triazole based bis-N-heterocyclic carbene ligands and their ruthenium complexes. The new water soluble ruthenium(II) complexes showed excellent catalytic activity in transformation hydrogen reaction. The synthesis, characterization and catalytic application of new water soluble metal complexes will be presented.

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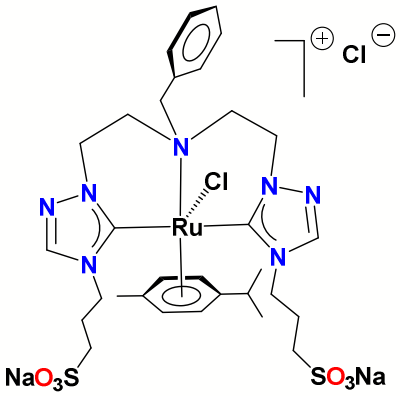

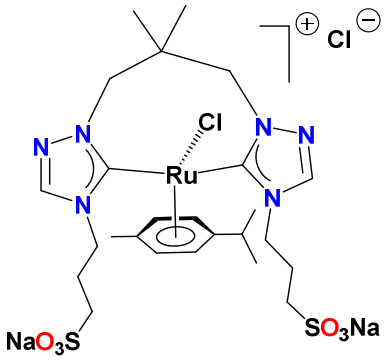

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Bis(pyrrolyl)pyridine based NNN-pincer palladium(II) complexes for catalyzing Suzuki-Miyaura cross-coupling reaction in aqueous medium

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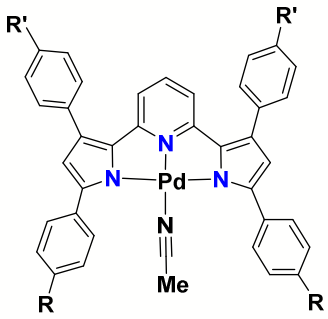
The reactivity of metal complexes is highly dependent on interaction between metal centers and their surrounding ligands. Ligands play a prominent role in the mechanism of catalytic system and allow for influence the reactivity and selectivity through steric and/or electronic properties of the metal center during the catalytic cycle [1-3]. Pincer based ligands are one of the most extensively used ligands for complexation with transition metals in organometallic chemistry. These ligands are powerful tools for catalysis in organic synthesis [4]. Along these lines, we have synthesized and characterized three new 2,6-bis(pyrrolyl)pyridine based [NNN]-pincer palladium(II) complexes (**1-3**). The complexes **1-3** have been synthesized from the reaction of corresponding pincer ligands with $Pd(OAc)_2$in acetonitrile in that acetonitrile bind to the palladium as labile group.The palladium complexes **1-3** showed efficient catalytic activity in Suzuki-Miyaura cross-coupling reaction in aqueous medium. Here in, the synthesis and catalytic application of these new palladium pincer complexes will be presented.



R = H, R' = OMe (**1**)
R = R' = OMe (**2**)
R = R' = Cl (**3**)

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P-205

Modification of Catalytic Activity of Myoglobin by Incorporating an Unnatural Amino Acid through Genetic Engineering.

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ABSTRACT:

With the incorporation of an unnatural amino acid in the amino acid chain of myoglobin (Mb) through genetic engineering, it was intended to induce the peroxidase activity. Here, in this study we replaced the H64 with a smaller residue, glycine. The expected distance between the new glycine residue and the heme iron center is estimated to be equal to that of cytochrome *c* peroxidase (C*c*P). Also, we mutated the leucine residue at the 29th position (L29) into an amber codon for incorporation of an unnatural amino acid [dihydroxy-L-phenylalanine (DOPA)]. Our results show that the presence of DOPA in the active site provides novel structural and functional properties to the mutant Mb. Our L29-DOPA/H64G mutant catalyzed the reaction between thioanisole and H_2O_2 to form the radical products -- biphenyl, diphenyl sulfide and diphenyl disulfide in addition to the expected mono-oxidized sulfoxide product. Moreover, we had immobilized L29-DOPA/H64G Mb on the L-cysteine modified Au electrode using EDC (1-Ethyl-3-[3-dimethylaminopropyl]carbodiimide) assisted reaction. The surface coverage ($\Gamma_{average}$) was 9.35 x 10^{-12} mol cm^{-2}, while the rate of heterogeneous electron transfer from the Au electrode to the iron center of the immobilized mutant Mb was observed to be 2.45 s^{-1}. Additionally, the electrocatalysis of ascorbic acid to its oxidized form was carried out by the immobilized mutant protein. Therefore our Au/L-Cys/L29DOPA H64G Mb electrode can be used as a sensor to detect ascorbic acid.

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P-206

Management of Saline Effluent Discharged from an Activated Clay Plant: Recovery of valuable chemicalsbased on iron and aluminium fromwaste

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Keyword: Industrial Effluent, calcium carbonate, ammonium carbonate, sodium hydroxide

Abstract: Clay plants release a huge amount of effluent enriched in inorganic metalions such as iron, aluminium and inorganics such as sodium, sulphate, calcium, magnesium and potassium etc. As a case study we have separated metal and inorganic ions using salts, acids or bases through phase equilibrium by adjusting pH of the effluent stream of a clay plant. Neutralization of effluent with pure NH_3 resulted in precipitation of salts rich in aluminium and iron while the neutralization with NaOH led to recovery of different salts selectively at different pH values. At pH 3.0 Fe rich salt was precipitated while at higher pH (4.5 and 7.2) Al based salt was selectively precipitated. Use of $CaCO_3$ also resulted in selective precipitation of Al and Fe based salts at different pH values. For further value addition, the effluent was treated with another effluent of a pigment industry which was enriched with ammonium carbonate $(NH_4)_2CO_3$. Ammonium carbonate effluent effectively precipitated different salts at different pH values leading to efficient management of both the effluent streams simultaneously. Salt precipitated have been analysed using volumetric, gravimetric, IC and ICP techniques. Morphology of precipitated salts have been investigated using FE-SEM.

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Fluorescence Quenching and Thermodynamic Parameters Study of Aloe-Emodin Complexation with Yeast-RNA

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Aloe-emodin (1, 8-dihydroxy-3-hydroxyl-methylanthraquinone) is a hydroxyanthraquinone found in the roots and rhizomes of *Rheum palmatum* and also in the leaves of *Aloe vera* [1, 2]. It has been extensively used for the studies of antiviral, anti-inflammatory, anti-diabetic, immunosuppressive, lung squamous cell carcinomas and anticancer activity [3, 4]. In this study fluorescence was employed to understand the binding and thermodynamic effect of the aloe-emodin with yeast-RNA. Aloe-emodin showed a strong fluorescence quenching of peak at 573 nm by the addition of y-RNA which confirmed the binding of aloe-emodin with y-RNA having binding constant of 3.88 x 10^4 mol^{-1}. Binding constant showed the intercalated binding mode of Aloe-emodin with yeast-RNA. The thermodynamic parameters Enthalpy change (ΔH), Gibbs free energy (ΔG), Entropy change (ΔS) at different temperature indicated that the hydrogen bonds, van der Waals interactions and hydrophobic interactions have a major role in the binding of Aloe-emodin with y-RNA at physiological pH. The results may provide a basis for further studies and clinical application of Aloe-emodin class of anticancer drugs.

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P-208

4-Aminoquinoline-Chalcone/-*N*-Acetylpyrazoline Conjugates: Synthesis and antiplasmodial Evaluation

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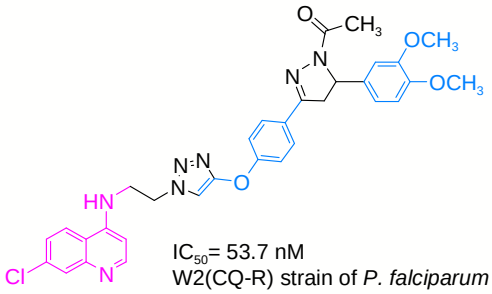
Abstract: 1*H*-1,2,3-triazole linked4-aminoquinoline-chalcone/-*N*-acetylpyrazoline conjugates were synthesized and evaluated against cultured chloroquine (CQ) resistant strain. Antiplasmodial activities of the synthesized conjugates revealed dependence of activity on the length of the alkyl chain as well as on the presence of methoxy substituents on ring A/ring B of the chalcone. The most potent and non-cytotoxic conjugate showed comparable antiplasmodial activity with that of CQ, with an IC_{50} value of 53.7 nM.[1]



IC_{50}= 53.7 nM
W2(CQ-R) strain of *P. falciparum*

Reference:

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P-209

Spectroscopic determination of some common anions in the light of dye surfactant interaction

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Abstract: Recently binary dye-surfactant systems paid widespread attention of scientific community due to their vast applicability in chemical sensing, biomedical and textile industries etc. In this context understanding the physiochemical interaction between dye and surfactant becomes acute need for proper application of these binary systems. In our present study we consider an anionic surfactant (sodium dodecyl sulphate) -cationic dye system for insight the molecular level interaction both in aqueous and organic medium. Well developed spectroscopic method like UV-visible and fluorescence techniques were considered for study the photochemical activity of dye in organized miceller media. The incorporation of dye molecules as a probe onto micellar system was confirmed from change of micellar system's conductance and spectral characteristics of dye. Additionally we have studied the effect of different anionic additives on the physiochemical activity of present dye-surfactant system. Time resolved fluorescence technique was utilized to detail understanding the molecular level interactions. The charge of anion found to be a major contributor for determining the photochemical activity of present binary system. Present study could provide a new dimension to develop dye-surfactant based future chemosensor.

Key words: dye, surfactant, miceller media.

P-210

Metal-free synthesis of polysubstituted pyrroles using surfactants in aqueous medium‡

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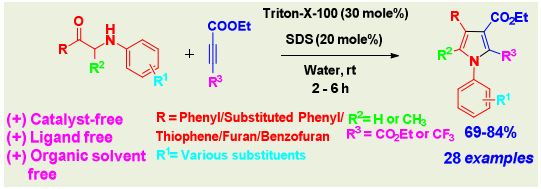
Abstract: An efficient and metal free method has been developed for the synthesis of polysubstituted pyrrole derivatives via intermolecular cyclo addition of substituted 1-phenyl-2-(phenylamino)-ethan-1-one /1-phenyl-2-(phenylamino)-propan-1-ones/ 2-((4-methoxyphenyl)amino)-1-(thiophen-2-yl)ethan-1-one/1-(furan-2-yl)-2-((4-methoxyphenyl)amino)ethan-1-one/ 1-(benzofuran-3-yl)-2-((4-methoxyphenyl)amino)ethan-1-one and dialkyl acetylene dicarboxylate/ethylbutynoate in the presence of combination of sodium dodecyl sulphate (SDS) and triton X-100 surfactants using water as a solvent at room temperature in 2-6h and microwave conditions (10 min) with good to excellent yields.



Key words:**1**-Phenyl-2-(phenylamino)-ethan-1-one (α-amino ketone), Dialkyl acetylene carboxylates, intermolecular cycloaddition, sodium dodecyl sulphate, triton X-100 and metal free synthesis.

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P-211

Antimicrobial potential of thiodiketopiperazine derivatives produced by *Phoma* sp., an endophyte of *Glycyrrhiza glabra* Linn.

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Abstract

During the screening of endophytes obtained from *Glycyrrhiza glabra* Linn., the extract from a fungal culture designated as GG1F1 showed significant antimicrobial activity. The fungus was identified as a species of the genus *Phoma* and was most closely related to *Phoma cucurbitacearum.* The chemical investigation of the GG1F1 extract led to the isolation and characterization of two thiodiketopiperazine derivatives. Both the compounds inhibited the growth of several bacterial pathogens especially that of *Staphylococcus aureus* and *Streptococcus pyogenes*, with IC_{50} values of less than 10 µM. The compounds strongly inhibited biofilm formation in both the pathogens. *In vitro* time kill kinetics showed efficient bactericidal activity of these compounds. The compounds were found to act synergistically with streptomycin while producing varying effects in combination with ciprofloxacin and ampicillin. The compounds inhibited bacterial transcription/translation *in vitro*, and also inhibited staphyloxanthin production in *S. aureus*. Although similar in structure, they differed significantly in some of their properties, particularly the effect on the expression of pathogenecity related genes in *S. aureus* at sub-lethal concentrations. Keeping in view the antimicrobial potential of these compounds, it would be needful to scale up the production of these compounds through fermentation technology and further explore their potential as antibiotics using *in vivo* models.

Key words: licorice, *Glycyrrhiza*, *Phoma*, antimicrobial activity, biofilm disruption, endophyte, fungal secondary metabolite

P-212

Stimuli Responsive Peptide based Cationic Polymer-Polyoxometalate Supramolecular Nanocomposite with Altered Antimicrobial Mechanism

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Because of the increasing prevalence of multi-drug resistance feature, several investigations have been so far reported regarding the antibiotic alternative supramolecular bioactive agents made of hybrid assemblies.[1, 2] In this regard, it is well established that combinational therapy inherited by assembled supramolecular can improve the bioactivity to some extent but their mode of actions have not been studied in details. We provide the first direct evidence that the improved mechanism of action of antimicrobial supra-amphiphilic nanocomposites differ largely from their parent antimicrobial peptide based polymers. For the construction of hybrid combinational system we have synthesized side chain peptide based antimicrobial polymers via RAFT polymerization [3] and exploited their cationic nature to decorate supra-amphiphilic nanocomposites via interaction with anionic polyoxometalates. Due to cooperative antimicrobial properties both of polymer and polyoxometalates, the nanocomposites shows enhanced antimicrobial activity with different antimicrobial mechanism. The cationic stimuli responsive peptide based polymers attacks bacteria via membrane disruption mechanism whereas free radical mediated cell damage is the likely mechanism of polymer-polyoxometalate based supra-amphiphilic nanocomposites. Thus our study highlights the different antimicrobial mechanism of combinational systems in details which improves our understanding of enhanced antimicrobial efficacy.

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P-213

Fluorescent Probes for Monitoring Gaseous signalling molecules and Identification of Diseases

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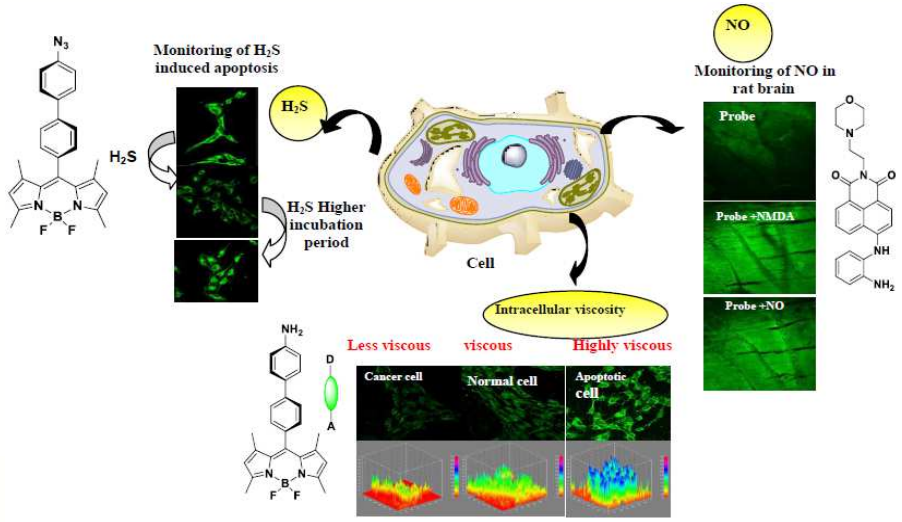
Recently, there has been a lot of interest in the development of fluorescent probes for bio-imaging and identification of diseases. In our body, diseases arise due to abnormal changes in gaso-transmitters (H_2S and NO) and intracellular viscosity. Thus, designing of fluorescent probes which can monitor gaso-transmitters and intracellular viscosity may acts as a tool for diagnosis of many diseases. In this context, we have designed a fluorescence probe for monitoring of H_2S induced apoptosis [1]. Here, we reported a dual functional strategy for the detection of H_2S and its anticancer effect in living cells. For monitoring of NO, we designed lysosome targetable probe which detects NO in living cells as well in rat brain tissue and explored its application in real field [2]. Further, for the diagnosis of diseases like cancer and apoptosis, we reported a smart strategy based on molecular rotation of *meso*-substituted bodipy [3]. Using this molecular rotor, we explored an easy and economical approach for identifying diseased cells out of normal cells on the basis of changes in intracellular viscosity.



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P-214

Some synthetic flavone derivatives acting as Topoisomerase –I poisons: A molecular modeling approach

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An important mechanism of action of anticancer agents is to target enzymes essential for cell proliferation. Topoisomerase-I is one such class of enzymes that relaxes supercoils generated in DNA by forming a nick in one DNA strand through formation of a transient covalent enzyme-DNA complex and religating it after releasing the torsional stress. Thus inhibiting topoisomerase –I can bring about significant changes in the cellular machinery. An important class of inhibitors are topoisomerase –I poisons which can stabilize these covalent adducts to prevent religation that eventually results in double strand breaks in DNA thus inducing cell death.

Flavones are well known for their varied biological activities- as antioxidants, anti-inflammatory, antimutagenic and anticancer properties. Our study involves the evaluation of topoisomerase-I inhibitory activities of some synthetic flavones using molecular modeling approaches. The results showed that all these molecules showed interactions with catalytically important amino acid residues like Asn352, Glu356, Arg364, and Asn722 of topoisomerase –I as observed in case of camptothecin, a known topoisomerase-I poison. They also showed interactions with some additional amino acid residues which are also present in the catalytic domain of topoisomerase-I. Mainly, the interaction with the tyrosine residue (Tyr723) which is involved in the nucleophilic attack at the phosphodiester DNA backbone could be significant for stabilizing the ligands binding to topoisomerase I / topoisomerase I –DNA complex to act as poisons.

Our findings are important in drug development for the potential therapeutic benefit in diseases like cancer.

P-215

Peptide based Stimuli Responsive Cationic Polymer as a Potential Drug-Delivery Vehicle with Antimicrobial Activity

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Application of peptide based cationic polymer is now an emerging area of research. Here synthesis and applications of a dipeptide based cationic polymethacrylate macromolecule would be presented. The monomer Boc-Lys-Phe-hydroxyethylmethacrylate (Boc-Lys-Phe-HEMA) has been synthesized and then applying reversible addition–fragmentation chain transfer (RAFT) polymerization technique followed by deprotection the final compound was obtained. It is water soluble and pH responsive in nature. Dynamic light scattering (DLS) and scanning electron microscope (SEM) study confirmed the formation of nanostructure aggregate upon self-association in aqueous solution. These nanostructure aggregates have the ability to encapsulate an anticancer drug Doxorubicin. The pH responsiveness leads the controlled release of encapsulated drug with high potential. In vitro cytotoxicity assay reveals very low toxicity of the polymer. The positively charged surface of the aggregated polymer has been utilized to assess antimicrobial feature. Finally, this cationic biocompatible polymer has ability to form polyplexes with DNA with an enzyme responsive decomplexation feature.

P-216

Acridine derivative interacts with DNA to sensitize human melanoma cells to ultraviolet A radiation

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Acridines are an important class of bioactive compounds that have proven anti-protozoal, antibacterial and anticancer properties. The phenyl derivatives of acridines are less well explored. Our laboratory has been engaged in studying the anticancer activity in some of these molecules.

Most often, acridines exert their action through their DNA binding affinity. We have therefore studied the interaction of 9-phenylacridine (ACPH) with calf thymus DNA *in vitro* through biophysical techniques and molecular docking studies through absorption titration assays, thermal denaturation, viscometry, displacement assays and also from molecular docking. ACPH binds to DNA both through intercalation and groove-binding. The stoichiometry of binding was found to be 1:4 with a K_b value of the order of ~10^3. and the interaction was primarily non-ionic.

We also investigated the effect of ACPH treatment on the sensitivity of cells to ultraviolet A radiation (UVA).We found that pretreatment of A375 cells, human melanoma cell line, with a non-toxic dose of ACPH resulted in sensitizing the cells to killing by UV-A light. We evaluated cell viability, DNA damage, generation of ROS, lipid peroxidation, glutathione content, mitochondrial membrane potential, induction of apoptosis and melanin production. Our results indicated that through binding to DNA, ACPH can act as a photosensitizer.

Our findings are important as it indicates the potential of ACPH in photodynamic therapy of cells having proliferative disorders, most importantly skin cancer.

P-217

VOLUMETRIC AND VISCOMETRIC PROPERTIES OF L-LEUCINE IN AQUEOUS CITRIC ACID SOLUTIONS AT DIFFERENT TEMPERATURES

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Apparent molar volumes (ϕ_v) and viscosity B-coefficients for L-Leucine in water and in aqueous (0.1, 0.3 and 0.5) M citric acid (CA) at different temperatures have been determined from experimental density and viscosity (η) measurements. Partial molar volumes (ϕ_v^o) have been evaluated together with partial molar volumes of transfer, $\Delta_{tr}\phi_v$ from water to aqueous CA solutions. Volumetric interaction coefficients (V_{AB} and V_{ABB}) indicate the interaction of L-Leucine in water and in aqueous CA solutions. The results obtained have been discussed in-terms of solute-solute and solute-solvent interactions which increase with increase in solvent concentration.

P-218

INTERACTIONS OF GLYCINE WITH AQUEOUS SOLUTIONS OF SODIUM/POTASSIUM PHOSPHATE BUFFER AT DIFFERENT TEMPERATURES

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ABSTRACT: Interactions of glycine with sodium/potassium phosphate buffer have been investigated by volumetric studies. Densities have been measured for glycine in water of different pH and in varying concentrations of aqueous sodium/potassium phosphate buffer solutions as a function of concentration at T = (288.15 to 328.15) K and at different pH values by using digital density meter. Apparent molar volumes ($V_{\emptyset}$) and partial molar volumes (V_2^o) obtained from these density data have been used to calculate partial molar volumes of transfer ($\Delta_{tr}V_2^o$), which are positive for zwitterionic and deprotonated form of glycine. Interaction coefficients have been obtained from$\Delta_{tr}V_2^o$ data. It has been observed that potassium phosphate buffer has higher tendency towards pair-wise interactions than sodium phosphate buffer. Effect of temperature on these thermodynamic properties have been studied by determining the partial molar expansibilities $(\partial V_2^o/\partial T)_P$and their second order derivative $(\partial^2 V_2^o/\partial T^2)_P$ at different temperatures and at different pH values. Hydration number (n_H) of glycine at pH 7.40 have been determined from the V_2^o data. The results have been rationalized in terms of various interactions taking place in these systems.

P-219

Potential Triterpenoids From *Ziziphus mauritiana* Lam Root For Evaluation of Paracetamol Induced Hepatotoxicity.

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Abstract

Objective: To evaluate the hepatoprotective activity of *Ziziphus mauritiana* root extract against paracetamol induced hepatotoxicity.

***Materials and methods*:** The ethanolic extract was obtained by continuous soxhlet extraction with methanol. The extract was concentrated, dried under vacuum and subjected to preliminary qualitative chemical investigation. From the above extraction two different compounds were isolated. They were designed as maslinic acid, 2α-hydroxyrosilic acid and betullinic acid. Further these isolated compounds were screened for hepatoprotective activity using rats (200-250 g) of either sex. A control group was treated with paracetamol orally by suspending in 5 % CMC . Hepatotoxicity was induced by administrating paracetamol (3mg/kg), silymarin (25mg/kg) a marketed product was taken as standard and other groups were treated with maslinic acid, 2α-hydroxyurosilic acid and betullinic acid. After 3 days the same serum was analyzed for alanine aminotransferase (ALT), aspartate aminotransferase (AST), alkaline phosphate (ALP) and bilirubin.

***Results*:** The hepatic enzymes ALT, AST, ALP and bilirubin in serum was significantly ($P<0.01$) increased in paracetamol treated animals when compared to control. maslinic acid and 2α-hydroxyurosilic acid exhibited more significantly ($P<0.01$) decreased the levels of AST, ALP and bilirubin ($P<0.01$) and ALT ($P<0.01$) when compared to control. Whereas betullinic acid showed moderate significant ($P<0.05$) activity. Silymarin (25mg/kg) treated animals also showed significant decrease in AST ($P<0.01$), ALT, ALP and bilirubin ($P<0.01$).

Conclusion: It was concluded from the result that, the maslinic acid and 2α-hydroxyurosilic acid exhibited more significant ($P<0.01$) hepatoprotective activity, whereas betullinic acid showed moderate activity ($P<0.05$) against paracetamol induced hepatoxicity in rats.

P-220

Thermodynamics investigations of L-threonine and DL-α-aminobutyric acid in aqueous 1-butyl-3-methylimidazolium bromide solutions at different temperatures

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ABSTRACT: Apparent molar volumes, $V_{\emptyset}$ L-threonine and DL-α-aminobutyric acid in pure water and in aqueous solutions of imidazolium based ionic liquid, 1-butyl-3-methylimidazolium bromide, $[BMIm][Br]$ were determined from precise density measurements at temperatures T = (288.15-318.15) K and at atmospheric pressure. Partial molar volumes, V_2^o follow the order: L-threonine > DL-α-aminobutyric acid. Positive partial molar volumes of transfer,$\Delta_{tr}V_2^o$ indicate the dominance of hydrophilic-ionic interactions between L-threonine/DL-α-aminobutyric acid and $[BMIm][Br]$. The partial molar expansibilities$(\partial V_2^o/\partial T)_P$and their second order derivatives $(\partial^2 V_2^o/\partial T^2)_P$, volumetric interaction parameters, V_{AB} andV_{ABB}, hydration number, n_H have been calculated. The results have been interpreted in terms of possible interactions.

P-221

Synthesis of new photoproducts during the Photochemical reactions of 2-(furan-2-yl)-3-hydroxy-4*H*-chromen-4-one and 3-hydroxy-2- (thiophene-2-yl)-4*H*-chromen-4-one in cyclohexane and acetonitrile as solvent.

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Abstract

Photolyses of titled chromenones have been carried at their longest absorption band (~360 nm) using cyclohexane (CH) and acetonitrile (ACN) as solvents, in both the aerated and the de-aerated solutions. Different dimeric photoproducts are formed with both chromenones in aerated solutions. On photolysing 2-(furan-2-yl)-3-hydroxy-4*H*-chromen-4-one (**FHC)** in aerated cyclohexane, 2-(furan-2-yl)-2-{[2-(furan-2yl)-4-oxo-4*H*-chromen-3-yl]oxy}- 2*H*- chromene-3,4-dione (dehydrodimer) and on photolysing 3-hydroxy-2-(thiophene-2-yl)-4*H*-chromen-4-one (**THC)** in aerated ACN a different dimeric product has been isolated and identified. Corresponding 3-aryl-3-hydroxy-1,2-indandiones have also been detected with FHC in ACN and with THC in CH, in addition to the dimeric products in both cases. On the other hand, in de-aerated solutions only corresponding 1,2-indandiones have been detected. 3-(furan-2-yl)isobenzofuran-1(3*H*)-one as a secondary product has also been detected with FHC in both the solvents. An attempt has been made to isolate the spectra of photoproducts in situ. Excited State Intramolecular Proton Transfer (ESIPT) and Excited State Intramolecular Charge Transfer (ESICT) processes complicates the photo dynamics of the reaction and so makes it difficult to predict the mechanisms of the photo reactions. However, tentative mechanisms have been proposed for the formation of photoproducts. This work will be presented in a poster during the international conference held at Manipal University, Jaipur.

P-222

Green synthesis of gold nanoparticles using using *Crocus Sativus* (Saffron) and effect of cetyltrimethylammonium bromide on the morphology

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Sugar based bola bio-surfactant, Crocin, was used as a reducing and capping agent to the one pot controlled green synthesis of gold nanoparticles (AuNPs). UV–visible absorption spectra showed one surface plasmon resonance peak (SPR) at 570nm attesting the spherical crocin-capped AuNPs formation. Very tiny (quantum dots) spherical mono-dispersed and aggregated AuNPs were revealed by the transmission electron microscopic (TEM). Upon addition of CTAB the morphology changes drastically to triangular, truncated triangular and hexagonal gold nano-disks. Scanning electron microscopy (SEM) and energy dispersion X-ray spectroscopy (EDX) ascertain the surface morphology and elemental analysis of the synthesized gold nanoparticles. XRD and selected area electron diffraction (SAED) ring patterns reveal the crystalline nature and structure of AuNPs as face centered cubic (fcc). The complex formation between aqueous solution of gold salt and CTAB were also characterized by the conventional techniques. Polar head groups of Crocin, gentiobiose disaccharide, are responsible to the reduction of $HAuCl_4$ into the metallic gold.

Key words: Crocin; Aggregation; Gold nanoanisotrops; Morphology; Bola surfactant.

P-223

Diversity-Oriented Synthesis of Spirooxindoles Using Surface-Modified TiO_2 Nanoparticles as Heterogeneous Acid Catalyst

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Abstract

An efficient and diversity oriented synthetic protocol has been presented to synthesize spirooxindoles using isocyanide based multicomponent reaction in the presence of surface modified TiO_2 nanoparticles as recyclable and reusable heterogeneous acid catalyst. This convergent synthetic protocol incorporates structural complexity and molecular diversity in molecular structures with atom economy, synthetic efficiency and operational simplicity in a time and cost-effective manner. The recyclability and reusability of the catalyst make the present synthetic protocol economically viable for industrial processes.

Keywords: Groebke–Blackburn–Bienaymé reaction, Heterogeneous catalysis, Multicomponent reactions, Pictet–Spengler reaction, Spirooxindoles.

P-224

Efficient and green synthetic protocol for the synthesis of structurally diverse spiroheterocycles using GAAS as catalytic solvent

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Abstract

Diversity oriented efficient and green synthetic protocol has been reported for the synthesis of structurally diverse spiroheterocycles incorporating medicinally privileged heterocyclic substructures. The present synthetic protocol involves the tandem reaction of hydrazine hydrate, 3-aminocrotononitrile, isatins and carbonyl compound using GAAS as environmentally benign and sustainable catalytic solvent.

Keywords: chromenopyrazolopyridine, diversity oriented synthesis, environmentally benign synthetic protocol, indenopyrazolopyridine, pyranopyrazolopyridine, spiroheterocycles, GAAS.

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GRAFTING OF METHYL ACRYLATE ONTO SODIUM ALGINATE USING CERIC AMMONIUM NITRATE AS REDOX INITIATOR

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ABSTRACT: Unreported graft copolymer of poly methyl acrylate (PMA) with Sodium Alginate was synthesized by using ceric ammonium nitrate as a redox initiator, in an aqueous medium. The optimal reaction conditions for affording maximum percentage of grafting were evaluated by successively varying various reaction parameters such as concentrations of nitric acid, ceric ammonium nitrate, monomer (PMA) as well as reaction time, temperature and amount of substrate. The optimal reaction conditions for ceric induced grafting were : SA = 1.5 g (dry basis); [CAN] = 0.05 mol.L^{-1}; [HNO_3] = 0.30 mol.L^{-1}; [MA] = 0.304 mol.L^{-1}; Time = 2 h; Temperature = 40^0C and Total Volume = 150 mL At optimum grafting reaction conditions, the maximum values of the grafting yields achieved were %G = 230.55 and %GE = 97.31. The spectroscopic (FTIR), scanning electron microscopy (SEM) are used to characterize the samples. The synthesized graft copolymer, SA-g-PMA which may find its potential application as a metal adsorbent.

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Synthesis, biological evaluation and molecular docking of novel flavonoid-thiazolidinedione derivatives as α-glucosidase inhibitors

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Diabetes Mellitus (DM), as a metabolic disease is a growing health problem occur because of insulin secretion failure orinsulin resistance. Chromone and its derivatives are pharmacologically active compounds, having immense medicinal significance and known to exhibit a broad spectrum of therapeutic activities including antidiabetic.α-Glucosidase is a key membrane-bound enzyme in carbohydrate digestion, located in the epithelium of the human small intestine which hydrolyzes the terminal, non-reducing 1,4-linked α-D-glucose residues with release of α-D-glucose and helps digestion and absorption of sugars. α-Glucosidase inhibitors act drug for the treatment type-2 diabetes because they can lower the rate of carbohydrate absorption and suppression of postprandial hyperglycemia.A novel series of 2-Methylchromonyl linked para/meta benzylidene based thiazolidinedione (TZD), and their cyclic analogs rhodanine (RHD), hydantoin (HyD), thiohydantoin (THyD) were synthesized, characterized and evaluated for their α-amyloglucosidase inhibitory activity. The docking studies at the crystal structure of protein (PDB code: 3TOP) using SYBYL 7.3 (SYBYL 2006, available in our in silico Drug Design Laboratory) were carried out for prediction of binding affinities and interactions of the targeted new chemical entities as compared to the standard Acarbose.

P-227

Study of Rheological Behavior of Methyl Cellulose in relation to Long Chain Anionic Surfactants in presence of a Hydrophobic Drug.

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The interaction of Methyl Cellulose with anionic surfactants having different hydrophobic chain length with same head groups has been investigated through surface tension and rheological parameters. Also, the effect of hydrophobic drug Rifampicin on the surface tension properties and rheological behavior of polymer-surfactant solutions was studied. Rifampicin being susceptible to oxidation limits its usage. The formulated systems were employed to curb the unstability of Rifampicin to oxidation and degradation kinetics in the surfactant and polymer-surfactant systems was studied by using UV-spectrophotometry.The steady state bulk rheological experiments indicate that the addition of surfactants induce non-Newtonian behavior to the polymer. The effect of Rifampicin is that the viscosity in case of Sodium StearoylSarcosinate system decreases while as in Sodium LauroylSarcosinate, the viscosity remains unchanged. The oscillatory rheological experiments revealed that the gelation is dependent upon the frequency applied and the StearoylSarcosinate imparts more viscoelasticity than LauroylSarcosinate to the polymer solution. Moreover, in presence of Rifampicin, the viscoelastic character gets increased. Thermal gelation of MC as a function of surfactant concentration with and without rifampicin was also studied which revealed that StearoylSarcosinate does not raises much the gelation temperature than LauroylSarcosinate.

P-228

Investigation of the energy transfer as FRET between Pyrene, Coumarin480 and rhodamine6g in SDS and bmimDS.

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We investigated the effect of head group on the transfer of energy from Pyrene to Coumarin 480 and from Coumarin 480 to rhodamine6g pairs both independently and in co-solubilized state of all the three flourophores in two micellar systems of SDS and bmimDS. There is an efficient overlap between the emission and absorption spectra of both the pairs which is a necessary criterion for the occurrence of energy transfer as FRET (Fluorescence Resonance Energy Transfer). This gives an opportunity to study three level FRET from primary donor Pyrene to final acceptor rhodamine6g via coumarin 480 upon proper excitation. Upon solubilizing simultaneously all the three flourophores in SDS and bmimDS, transfer of energy takes place from Pyrene to rhodamine6g via Coumarin480, excited at the excitation wavelength of the primary donor Pyrene. The fluorescence intensity of rhodamine6g increased when the excited at 334 nm in presence of coumarin480 which is opposite to what is observed in absence of pyrene, confirming the transfer of energy from pyrene to rhodamine6g via coumarin480 (Figs 1and 2). The results were confirmed by the time resolved fluorescence measurements, wherein Rhodamine6g didn't show any increase in the lifetime in presence of coumarim480 at the excitation wavelength of 336 nm. The increase in the lifetime of rhodamine6g was observed to be 1.10 ns in case of bmimDS while in SDS it is 0.7 ns which is in complete conformity with the results from the steady state data. The efficiency of FRET in bmimDS is more than in SDS because of the smaller size and higher zeta potential of the former micelles.

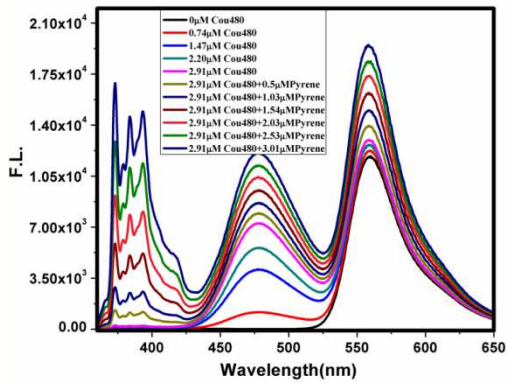

Figure 1

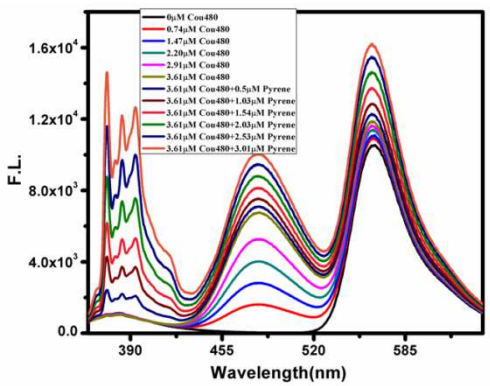

Figure 2

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Synthesis of selective 2-(furan-2-yl)-3-hydroxy-4*H*-chromen-4-one(FHC) derivatives for spectral studies in different solvent system

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In the literature different synthetic methods are reported for the synthesis of chromenones. In the present study we have selected two step method for the synthesis of chromenones. First step involves the condensation of differently substituted hydroxyacetophenones and 2-furaldehyde in the alcoholic solution. Second step is the oxidation of separated chalcones of previous step under algar-flymnoymada reaction conditions. After that identification and characterisation was carried out using different spectroscopic techniques like IR, H^1-NMR, EIMS etc. Then their spectral (absorption and emission) studies have been carried out in different solvents like cyclohexane, acetonitrile and methanol. These solvents differ from each other in their polarity, dielectric constant, H-bond donor and accepting ability. So, effects of these properties have been counted on spectral studies of substituted FHC chromenones.

P-230

MICROWAVE-ASSISTED FACILE SYNTHESIS OF BIOLOGICALLY ACTIVE THIAZOLO-PYRAZOLINES USING SOLID-SUPPORT

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We herein communicate the synthesis of "thiazolo-pyrazoline" scaffold using solid-support. Thiazoles and pyrazolines individually or in combination are associated with wide spectrum of pharmacological applications. As literature is flooded with such synthetic procedures which are associated with multi-step synthetic routes, longer reaction times, difficult work-up and utilization of expensive and hazardous chemicals.

With increasing community concerns over possible influence of toxic chemicals and practices associated with such chemicals on environment and present economic conditions; we have synthesized entitled organic moieties using principles of "Green Chemistry".

The desired products have been prepared using microwave-irradiations using solid support.

The synthesized moieties have been screened for their anti-microbial activities as well. Serial tube Dilution method has been employed and MIC (minimum inhibitory concentration, µg/mL) has been obtained for the prepared samples. Amoxicillin and Fluconazole have been used as standard drugs for carrying out anti-bacterial and anti-fungal activities respectively. And it was found that methyl substituted product showed the most potent anti-bacterial activity against *Staphylococcus aureus* among all the tested strains; at MIC 4 µg/mL, comparable to that of standard drug.

P-231

Quantitative Determination of Heavy Metals in Some Commonly Consumed Herbal Medicines in Kano State, Nigeria

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Abstract

Evaluation of heavy metals in twelve commonly consumed herbal medicines/preparations in Kano State Nigeriawas carried out. The samples comprised of five unregistered powdered medicines, namely, Zuwo (ZW); Rai Dorai, (RD); Miyar Tsanya, (MTS); Bagaruwar Makka, (BM); and Madobiya, (M); five unregistered liquid herbal medicines concussions for pile (MB), yellow fever (MS), typhoid (MT), stomach pain (MC), sexually transmitted diseases (STDs) and two registered herbal medicines; Alif powder (AP) and Champion Leaf (CL). The heavy metals evaluation was carried out using Atomic Absorption Spectrometry (AAS) and the result revealed the concentration (ppm) ranges of the heavy metals as follows: Cadmium (0.0045 – 0.1601), Chromium (0.0418 – 0.2092), Cobalt (0.0038 – 0.0760), Copper (0.0547 – 0.2465), Iron (o.1197 – 0.3952), Manganese (0.0123 – 1.4462), Nickel (0.0073 – 0.0960), Lead (0.185 - 0..0927) and Zinc (0.0244 - 0.2444). Comparing the results in this work with the standards of the World Health Organization (WHO), the food and Agricultural Organization (FAO) and the permissible limits of other countries, the concentration of heavy metals in the herbal medicine/preparations are within the allowed permissible limits range in herbal medicines and their use could be safe.

Keywords: Herbal medicines, Registered, Unregistered, Kano State

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SYNTHESIS, CHARACTERIZATION AND ANTIOXIDANT STUDIES OF A SERIES OF NOVEL 3-ARYL-1-PHENYL-1H-PYRAZOLE-4-CARBALDEHYDE-ACYLHYDRAZONES

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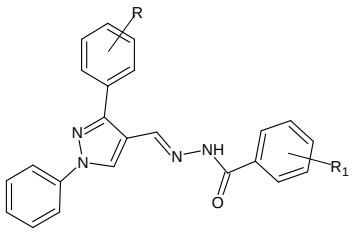
Abstract: Pyrazole derivatives occupy a distinct position in heterocyclic chemistry and serve as a key motif in medicinal chemistry due to their wide range of pharmacological activities. Various biologically important activities of pyrazole derivatives such as anti-inflammatory, analgesic, anti-fungal and anti-bacterial activities have been reported by Penning et al.[1], Menozzi et al. [2], Sridhar et al. [3] and Tanitame et al. [4] respectively. Sui et al. [5] have also reported the pyrazoles bearing 1,3- disubstituted aryl moieties with promising effect in COX-2 inhibition. Based on these observations on the development of new biologically potent pharmacophores, a series of new 3-Aryl-1-phenyl-1H-pyrazole-4-carbaldehyde-acylhydrazones **1** were synthesized and characterized by IR, LCMS and NMR techniques. Substituted 3-Aryl-1-phenyl-1H-pyrazole-4-carbaldehydes were synthesized by employing Vilsmeier-Haack reaction to the substituted phenylhydrazones using $POCl_3$ and dimethylformamide according to the procedure reported by Li et al. [6]. The title compounds were in turn synthesized by the reaction of these compounds with substituted benzoic acid hydrazides using ethanol as the solvent as reported by Bansal et al. [7]. The synthesized compounds were evaluated for their anti-oxidant properties using DPPH radical scavenging assay.



1

Keywords: Vilsmeier-Haack reaction; DPPH radical scavenging; pyrazole carbaldehydes; acid hydrazides.

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Synthesis, biological evaluation and molecular docking studies of novel benzimidazole derivatives as *α*-glucosidase inhibitors

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A novel series of **12** compounds N-substituted-benzimidazolyl linked *para*substituted benzyl based molecules containing three pharmacologically potent hydrogen bonding parts namely; 2,4-thiazolidinedione (TZD: a 2,4-dicarbonyl), diethyl malonate (DEM: a 1,3-diester and an isooxazolidinedione analog) and methyl acetoacetate (MAA: a β-ketoester) were synthesized and evaluated for their inhibitory action against *α*-amylase and *α*-amyloglucosidase.The structure of all the novel synthesized compounds was confirmed through the spectral studies (ESI-MS, ^{1}H-NMR, ^{13}C-NMR, FT-IR). Comparative evaluation of these compounds revealed that the compound **9b** with TZD as hydrogen bonding part showed maximum inhibitory potential against *α*-amylase and *α*-glucosidase giving an IC_{50} valueof 0.54 ± 0.01 µM. Furthermore, binding affinities in terms of G score values and hydrogen bond interactions between all the synthesized compounds and the AA residues in the active site of the protein (PDB code: 3TOP) to that of Acarbose (standard drug) were explored with the help of molecular docking studies. Compound **9b** was considered as promising candidate of this series.The work will be presented at 24th ISCB International Conference (ISCBC-2018) "**Frontier Research in Chemistry & Biology Interface-2018February 11th-13th, 2018"**

P-234

Bischromones: Synthesis and Characterization Studies

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Chromones are the important class of heterocyclic compounds containing benzopyran ring. These are widely distributed in natural products and interest in their chemistry continues because of their usefulness as biologically active agents. The bischromones have been prepared from the substituted 3-hydroxy-chromones-4-one with 4,4-bischloromethyldiphenyl in dry acetone, anhydrous K_2CO_3 and PTC ($Bu_4N^+I^-$) under refluxong conditions. The intermediates were obtained from the cyclization of the corresponding chalcones under the AFO reaction conditions. The chalcones were furthur obtained by the Claisen Schmidt reaction of the 5-methyl-2-hydroxyacetophenone with suitable aromatic aldehydes. IR, ^{1}H-NMR, ^{13}C-NMR & ESI-MS data were extensively used and ascertain the structures of the synthesized compounds. The antimicrobial activities of these bischromones were also evaluated against the selected number of bacterial and fungal strains.

P-235

Synthetic and Antimicrobial studies of new Bispyranopyrazoles

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Heterocyclic chemistry is an integral part of the organic chemistry and constitutes a considerable part of the modern researches. Pyranopyrazoles are the valuable heterocyclic compounds in which pyran and pyrazole moeity co-exist in the same molecule. These heterocycles are widely synthesized due their important biological applications. The bispyranopyrazoles required for the present study have been synthesized from one pot three component reaction of bisaldehyde, malononitrile and 3-methylpyrazole-5-one by refluxing under ethanolic medium. The structural framework of all the newely prepared bisheterocycles have been characterized from the analysis of their spectroscopic parameters like IR, ^{1}H-NMR, ^{13}C-NMR & ESI-MS. The antimicrobial activities of intermediates and final products were also evaluated against seven bacterial and five fungal strains. Most of the studied compounds exhibited moderate activity against the tested micro-organisms.

P-236

Expression analysis of the *Thermomyceslanuginosus* lipase gene

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Lipases represent the most widely used class of enzymes in biotechnological applications and organic chemistry as they bring about a wide range of bioconversion reactions. The increasing demand for thermostable lipases that can compete with the likes of CalB in terms of reactivity and stability, have paved the way for extensive research in this direction. Cloning and expression of lipases in mesophilic organism is reported, though yields of expressed protein are low and cannot meet the requirements of enzymes sold in the market (100KLU/gm of protein). Modern methods of genetic engineering with an increasing knowledge of structure and function will allow further adaptation to industrial needs and exploration of novel applications. Production of such tailored lipases require their functional overexpression in a suitable host.For a gene LIP from *Thermomyceslanuginosus*, coding for a triacylglycerol lipase was overexpressed in different hosts like *E.coli* and *Bacillus subtilis* (prokaryotic expression hosts) and *Yarrowialipolytica* (eukaryotic expression host) with the aim of looking for a host with high-volume/low-cost application in industry. The yield was found in the order as*Bacillus subtilis*, *E. coli*, *Yarrowialipolytica* (intracellular< extracellular expression) respectively.Currently, we are working on lowering the costs of production for meeting the cost requirements of commercial enzymes.

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GREEN APPROACH TO CORROSION INHIBITION OF LOW CARBON STEEL IN 1 M HYDROCHLORIC ACID SOLUTION BY THE GUM OBTAINED FROM *BOSWELLIA SERRATA*

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ABSTRACT

Boswellia serrata gum (BSG) was studied as a new sustainable green corrosion inhibitor for the protection of low carbon steel (LCS) in 1 M HCl solution employing standard experimental techniques. The corrosion behavior of LCS induced by BSG was studied using different techniques such as potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS) at different concentrations and 30º C temperature. The inhibition efficiency (%η) of LCS in 1 M HCl increase with an increase in inhibitor concentrations. As evidenced by PDP measurements BSG acted as mixed type inhibitor with dominant anodic effect. EIS results reveal that mitigation efficacy of BSG is due to the adsorption of the constituents polysaccharides on LCS surface and the process of their adsorption followed Langmuir adsorption isotherm. SEM/EDX results substantiated the inhibitive effect of adsorbed BSG constituents on the LCS surface. The result shows that BSG is good corrosion inhibitor for LCS in 1 M HCl solution.

Keywords: Boswellia serrata; Corrosion inhibition; Potentiodynamic polarization; EIS

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Palladium-Ag_2O catalyzed decarboxylative cross-coupling of alkynyl carboxylic acids with triarylbismuth reagents

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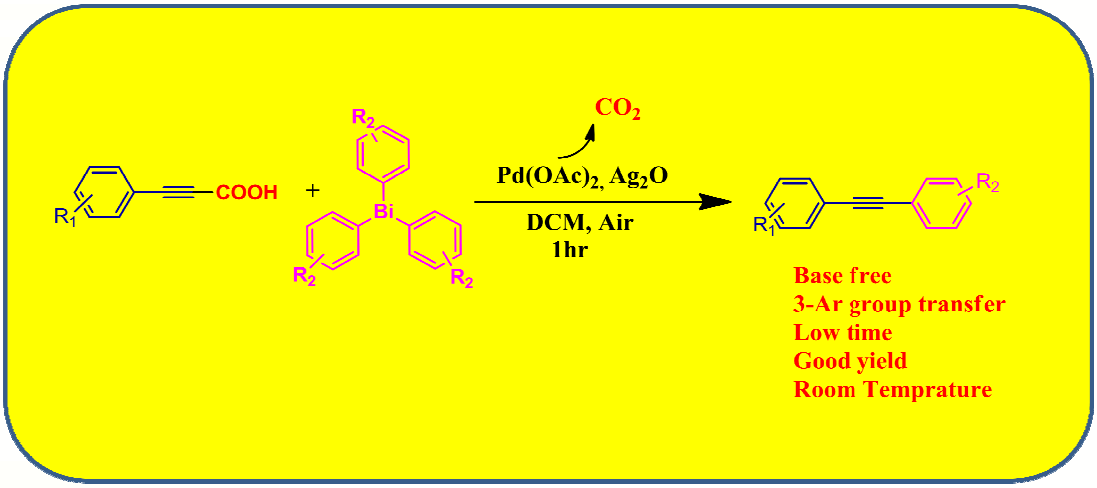
Abstract

In present work we describe a novel base free methodology for the decarboxylative cross-coupling reaction of alkynyl carboxylic acids with triarylbismuth reagents. The $Pd(OAc)_2$-Ag_2O homogeneous catalytic system used for the decarboxylative cross-coupling reaction. The reaction proceeds at room temperature with short reaction time. Triarylbismuth reagents used as threefold arylating reagent which is attractive due to their air and moisture stability, high functional group tolerance and threefold arylating property. This protocol is particularly useful for the synthesis of unsymmetrical substituted alkynes .

General Scheme



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Semisynthesis and biological evaluation of andrographolide and neoandrographolide analogues

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Abstract: Natural products have been a great source of pharmaceuticals since ages. Vast screening of natural products from different sources has led to the discovery of plethora of chemotherapeutic drugs and other compounds for the betterment of human life. Several bioactive entities have been generated by the structural modifications of the natural products or by using the natives as key models in synthetic chemistry. Nonetheless, a number of natural compounds with potential bioactivities remain unexploited in the medicinal field due to their stringent chemical properties. *Andrographis paniculata*, a traditional medicinal herb from family Acanthaceae is particularly known for its multiple pharmacological activities. It's major bioactive constituent "Andrographolide", possessing prominent anticancer potential is one such unexploited treasure [1]. It's architecture consisting of an α-alkylidene γ-butyrolactone moiety, two olefin bond [$\triangle^{8(17)}$ and $\triangle^{12(13)}$], three hydroxyls at C-3, C-19, and C-14 and highly substituted trans decalin. Of the three hydroxyl groups, one is allylic at C-14, and the others are secondary and primary at C-3 and C-19, respectively [2]. By modification of the above structural features a number of andrographolide derivatives have been synthesized [3]. The second principle phyto-constituent, 'neoandrographolide' of *A. paniculata* was explored to assess its semi synthetic derivatives for their antimicrobial potential.

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P-240

VALIDATION OF HPLC METHOD FOR DETERMINATION OF VEGETABLE OILSEED CAKE AMINO ACIDS

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Abstract: vegetable oil seed cake protein can be a medium to help resolve the shortage of food protein. The subject of this study was the validation of high-performanceliquid chromatography method for the analysis of amino acids in vegetable oil cake. Thecontents of amino acids were determined in Sunflower cake, Soybean cake, Rapeseed cake and Cottonseed cake. The main principle applied thatPrimary amines react readily with OPA in the presence of mercapto ethanol to form 1 thiosubstituted 2-alkyl isoindoles. These isoindoles have been shown to be well suited for HPLC separation. OPA derivatization procedures involve a rapid reaction and high sensitivity. The resultsdemonstrated that the procedure could be used as a method for the determinationof the composition of primary amino acids of vegetable oilseed cake proteins.This extracted proteins from vegetable oilseed cake can be a potential source of value added products for nutraceuticals, cosmeceuticals and surfactant applications.

Key words: Vegetable oil seed cake, Amino acids, Protein, HPLC method.

P-241

ECG Feature Extraction and Detection of First Degree Atrioventricular Block

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ABSTRACT— Electrocardiogram has been the most prominent diagnostic technique for cardiac disease detection. Electrocardiogram (ECG) is used to measure the rate and regularity of heart beats as well as the size and position of chambers. It helps cardiologist to obtain the waveform of heart electrical potential activates, which enables them in detecting several heart problems, such as arrhythmia, which is the leading cause of death. As the ECG monitoring is widely used in diagnostic, many challenges have been faced by patients due to lack of availability of cardiac specialists at remote areas or rural areas. It is not possible that the cardiologist with entire system of diagnosis to visit again and again to patient for monitoring of ECG.

Currently there are many computer based approach which employs certain signal processing to diagnose a patient based on ECG recording. The purpose of this research is to address in identifying the features of ECG and detection of first degree atrioventricular block. LabVIEW is used to extract the relevant information from the ECG input data which are Mean and Standard Deviation value. Then the extracted features data is analyzed and classified using LabVIEW program. The proposed system is implemented and also tested in LabVIEW software. The proposed system successfully extracted ECG features and classifies the first degree atrioventricular block with the rate of accuracy 97.22%.

INDEX TERMS— ECG, EEG, PCG, LABVIEW, AV, HPF

P-242

Identification of a Receptor-Binding Peptide Derived from Diphtheria Toxin

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Human Heparin-binding EGF-like Growth Factor (HB-EGF) is the receptor of Diphtheria toxin (DT). DT binds to HB-EGF on the cell surface and enters cells through receptor-mediated endocytosis. HB-EGF is overexpressed in various types of cancer and modulates oncogenic signaling. Therefore, HB-EGF is a good target for therapeutic purposes. In this work, we have identified a 26 amino acids long segment in DT that has a β-hairpin structure and makes multiple contacts with HB-EGF. Our molecular dynamic simulation and docking experiments showed that this region could form a stable β-hairpin and bind to the designated binding-groove on HB-EGF. We have synthesized this peptide by solid-phase synthesis and showed that this peptide binds HB-EGF. Furthermore, we tagged this peptide to maltose-binding protein (MBP) and expressed it as a recombinant protein. This recombinant MBP-tagged peptide binds to HB-EGF with a high affinity comparable to the affinity of DT for HB-EGF. This work shows that this particular a short stretch of 26 amino acids of DT is adequate for binding to HB-EGF, even in the absence of the rest of the protein. This peptide may also be used as a homing peptide to deliver small molecules or proteins to cells overexpressing HB-EGF on their surface.

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Tensiometric study of Dodecyl sulfate and dodecyl benzenesulfonate based ionic liquids with Polyelectrolyte – NaPSS

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Dodecyl sulfate and dodecyl benzenesulphonate having imidazolium as a cationic moiety, Ionic Liquids (IL) were synthesized and characterized by ^{1}H-NMR, thin layer chromatography. Interactions between these ionic liquids and Polyelectrolyte-NaPSS(Sodium polystyrene sulphonate) have been studied by Surface tension techniques at a fixed concentration of NaPSS. The surface parameters such as critical aggregation concentration (CAC), adsorption efficiency, surface pressure at the interface, surface tension at CAC, theminimum area occupied by asingle molecule, maximum surface excess concentration were calculated from surface tension measurements with and without salts. The results show that these ionic liquid forms aggregates at lower concentration and acts as abetter cationic surfactant.

KEYWORDS: Polyelectrolyte, Imidazolium based Ionic liquids, Surface Tension

P-244

Synthesis, characterization and biological evaluation of 4-oxo-thiazolidine compounds

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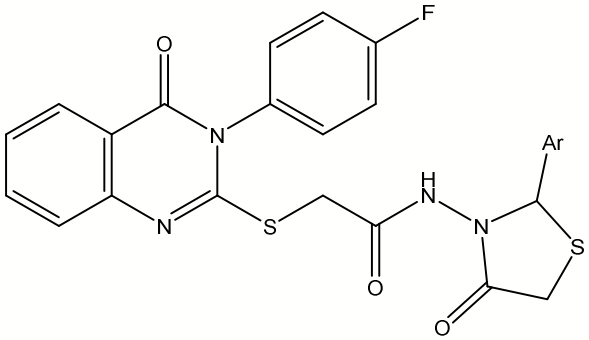
ABSTRACT:

The nucleus of 4-oxo-thiazolidine derivatives has occupied a unique place in the field of medicinal chemistry due to a wide range of biological activities[1,2]. A series of compounds 4-oxo-thiazolidine derivatives,N-(2-aryl-4-oxothiazolidin-3-yl)-2-((3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetamide (AJ5a–j)weresynthesized by condensation reactions[3]. The structure of synthesized compounds was characterized by IR, ^{1}H NMR, ^{13}CNMR and mass spectrometry. The present work deals with newly synthesized thiazolidine compounds AJ5a–AJ5j that were screened for their antimicrobial activity against different strains of bacteria and fungi using serial broth dilution method (Mueller–Hinton broth dilution method). *In vitro* antitubercular activity of compounds AJ5a–jwas carried out against Mycobacterium tuberculosis H37Rv. Compounds AJ5a, AJ5d, AJ5e, AJ5f and AJ5g were found most active against selected bacterial strains (MIC = 62.5µg/mL) and compounds AJ5a–jwas found moderately active against M. tuberculosis.

Keywords: 4-Oxo-thiazolidine, Antibacterial activity, Antifungal activity, Antitubercular activity



Where, Ar = Aromatic aldehyde.

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P-245

Defluoridation of Ground Water Using Activated Carbon of Ber (*Indian Jujube*) Leaves

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Abstract: The Present study deals with defluoridation of ground water using activated carbon of ber (*Indian jujube*) leaves. In this study, Activated Ber leaves carbon (ABLC) prepared by heating the leaves in electric furnace was found to be useful for the removal of fluoride. Batch experiments were applied on water sample to study the influence of pH, adsorbent dose and contact time on adsorption efficiency. Fluoride removal reached a maximum of 72.5% by particle size 0.3mm of ABLC at pH 6.0. The adsorption of fluoride from aqueous solution with ABLC followed Freundlich equation. The values of adsorption capacity (K) and intensity of adsorption (1/n) indicate greater affinity for fluoride. Thermally activated Ber leaves carbon (ABLC) was good adsorbent.

Index Terms— Defluoridation, Ground water, Adsorption, Ber leaves, Activated carbon

P-246

Design, Synthesis, and Screening of Triazolopyrimidine-Pyrazole Hybrids as Potent Apoptotic Inducer

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Keywords: 1,2,4-Triazolopyrimidine; Pyrazole; Hypervalent iodine; Apoptosis; Cytotoxic activity.

ABSTRACT

An efficient synthesis of novel 3-(3-aryl-1-phenyl-1H-pyrazol-4-yl)-5,7-dimethyl-[1,2,4]triazolo[4,3-a]-pyrimidines was accomplished by the oxidation of pyrimidinylhydrazones by using organoiodine(III) reagent. All new triazolopyrimidine derivatives bearing the pyrazole scaffold were screened to evaluate them as a reproductive toxicant in the testicular germ cells of goat (Capra hircus). This study aimed at assessing the cytological and biochemical changes in testicular germ cells after the exposure to triazolopyrimidines in a dose- and time-dependent manner. Histomorphological analysis, fluorescence assays, apoptosis quantification, and terminal deoxynucleotidyl transferase dUTP-mediated nick-end labeling (TUNEL) assays were performed to determine cytological changes, whereas thiobarbituric acid-reactive substance (TBARS) and ferric reducing antioxidant power (FRAP) assays were carried out to measure the oxidative stress in triazolopyrimidines treated germ cells. The parallel use of these methods enabled us to determine the role of triazolopyrimidines in inducing apoptosis as a consequence of cytogenetic damage and oxidative stress generated in testicular germ cells of goat.

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Comparative thermoanalytical and spectral studies of polyvinyl alcohol-carrot fiber composite thin films

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All over the world, the concern regarding many environmental problems including difficulties in waste disposal and global warming caused by nonbiodegradability of polymers have been raised. To reduce the problems caused by plastic waste, efforts have been made to prepare environmental friendly materials. Carrot (*Daucus Carota L.)* is one of the imperative roots vegetable. Carrot fiber consists of cellulosic substances and can be used to make eco-friendly and economical packaging films. Carrot residue in dry form contains 81% Cellulose, 9% Hemicelluloses, 2.5% lignin and 7.5% pectin. High cellulose content in carrot fiber makes it a potential reinforcement material in polymer composites. Thin films of Polyvinyl alcohol (PVA) reinforced Carrot fiber (CF) has been prepared by solution casting technique. The characterization of the prepared thin films has been carried out by Thermal analysis and UV-Spectra. Thermal decomposition of thin films was studied by thermogravimetric analyzer at a heating rate of 10°C/min in nitrogen atmosphere from ambient to 600°C. Kinetic parameters were calculated using single heating rate kinetic methods *viz.* Broido, Horowitz-Metzger and Coats-Redfern. Thermal stability and activation energy of the prepared thin films have been compared. An increase in absorbance intensity from UV-data is observed as the fiber content is increased. The clear shift of absorption edge upon addition of carrot fiber indicated the decrease in energy band gap.

Key words: Carrot fiber, polyvinyl alcohol, absorbance

P-248

Synergistic effect of Lycopene extracted from *Lycopersicon esculentum* with Ciprofloxacin against *Pseudomonas aeruginosa*

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Abstract: Synergism comes from Greek word "synergos" meaning working together i.e. interaction of agents, or condition such that total effect is greater than sum of their individual effects.The global focus is now on methods aimed at reducing drug dosage, and thus drug treatment cost. One way to achieve reduction in drug dosage, and therefore drug toxicity and cost, is to increase drug bioavailability.

Tomato is one of the most important vegetables worldwide because of its high consumption, year round availability and large content of health related components. Tomato contains a variety of phytochemicals such as lycopene, -carotene, vitamin- C, quercetin glycosides, and chlorogenic acid and have good health protective effects. It is also one of the most abundant non-vitamin analogues present in human blood from food consumption [1].Lycopene is one of about 600 naturally occurring carotenoids and is responsible for the red colour in fruits [2] . Lycopene has 13 double bonds, of which 11 are conjugated, resulting in excellent antioxidant properties. The presence of unsaturated bonds in its molecular structure make lycopene susceptible to oxidants, sensitive to light and heat. Because of its non-polarity, Lycopene is lipophilic, insoluble in water, and can be dissolved only in organic solvents and oils[3]. It is the most abundant carotenoid in tomatoes, followed by beta-carotene, gamma carotene and other minor carotenoids. The human body can not produce lycopene so it must be obtain from food sources.[4]The present work is to study synergism between lycopene and Ciprofloxacin *Pseudomonas aeruginosa*.

Keywords: lycopene ,synergism , extraction, Ciprofloxacin.

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P-249

Silica Supported-P_2O_5 as an efficient& Recyclable Catalyst for the Synthesis of Acridinediones in Solvent-free Conditions

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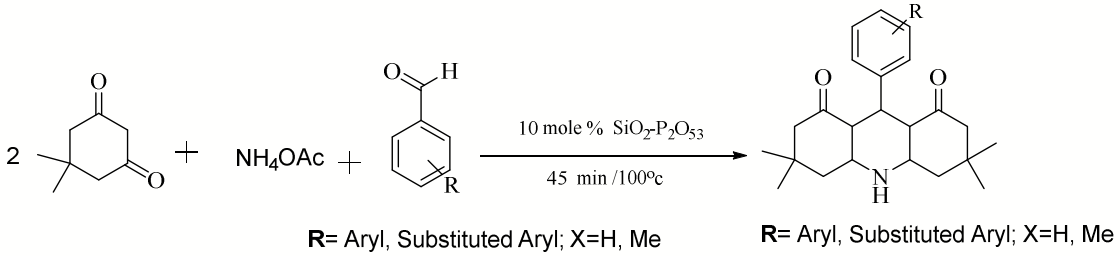
Presently Acridinediones have attracted eye-catching attention from around the world owing to its valuability in pharmaceutical as well in organic synthesis.Although literature is flooded with numerous methods including conventional thermal reactions, ionic liquid & microwave irradiation mediated along with other miscellaneous approaches. But the reported methods involves use of toxic catalyst as well as toxic solvent which are at the forefront to cause severe threaten to the environment. Thus to visualize the green chemistry concept we thought of developing a newer protocol that can fulfil the concept of green chemistry and hence we have performed the present reaction in solvent free conditions to avoid use of any toxic solvent.

A solvent-free approach has been introduced for the synthesis of acridinediones by the one pot three component reaction of Aromatic aldehyde, Dimedone and Ammonium acetate as a nitrogen source by recruiting Silica supported-P_2O_5 as a recyclable catalyst within 45 minutes of reaction time. The current protocol has many superior abilities like solvent-free, milder reaction conditions, recyclable, reusable, cheap & inexpensive catalyst, simple work-up procedure giving the product in excellent amount of yield. Further it works very well in terms of electron donating as well as electron withdrawing substituent containing aromatic aldehydes.



Scheme 1 : SiO_2-P_2O_5 Catalyzed Synthesis of Acredinediones

P-250

Preparation and evaluation of polyherbal gel in treating psoriasis

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ABSTRACT: The main objective of this study was to formulate and evaluate the polyherbal gel to treat psoriasis. Various formulations were prepared by using the extracts from the leaves of Azadiracta indica, Moringa oleifera and from the root powder of Withania somnifera. Prior to the formulation, these extracts were screened phytochemically to know the presence of alkaloids and flavonoids. These chemical constituents were responsible for anti-bacterial and anti-microbial activity.

Carbopol 934P is the polymer, which we have selected to develop polyherbal gel as it gives good stability. From the developed formulations F4 and F5 with carbopol concentrations 0.5% and 1% showed good results in comparison with marketed gel. The evaluated results like pH, consistency, spreadability, homogeneity, viscosity, appearance are satisfactory. Pathogenic microorganisms selected for microbiological assay includes two bacteria, viz., *Pseudomonas aeruginosa* (MTCC 2863), *bacillus subtilis* (MTCC 121) and one fungal strain viz., *Aspergillus niger* (MTCC 961). Bacterial strains were grown and maintained on "Muller- Hinton Agar Medium" while fungal strains were kept on "Potato Dextrose Agar Medium". These anti-microbial assays showed greater zone of inhibition compared to marketed gel. Skin irritation studies were also conducted on albino rats weighing 150-200gm which showed positive results. The optimized formulations were subjected to stability studies for three months as per ICH guidelines at 40^0 C ± 2^0C/ 75% ± 5% RH. The formulations were found to be stable with in significant changes in pH, consistency, spreadability, homogeneity, viscosity, appearance, microbiological assay and in invivo studies.

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P-251

Microwave assisted synthesis and biological screening of Ofloxacin derivative and its metal complexes

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Abstract: In this paper we present microwave assisted synthesis of Ofloxacin derivative with benzil dihydrazone in methanolic solution. Its divalent transition metal complexes have been derived by using chloride salt of cobalt, copper, nickel and zinc. The ligands and its complexes were characterized by with the help of physicochemical methods such as solubility, melting point, elemental analysis and various physicochemical techniques such as infrared, ^{1}H-NMR electronic spectra, UV, and molecular weight determination. On the bases of these studies, a six coordinate geometry proposed for all the metal complexes. . The synthesized ligand along with their metal (II) complexes were investigated for their in vitro antibacterial activity against gram positive bacteria Bacillus cereus and gram negative bacteria Escherichia coli using disk diffusion method. Among the all synthesized complexes copper complex was found remarkable antibacterial activity as compare to Ofloxacin.The synthesized ligand and its complexes were also screened for their antioxidant activity by using DPPH method.

Key words: Ofloxacin, benzil dihydrazone, Bacillus cereus, Escherichia coli , antioxidant activity, DPPH.

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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 introducediethanolamine group in epoxyalantolides ,isoalantolactone&alantolactone were allowed to reactwith an excess of perbenzoic acid followed by diethanolamine. In order to prepare more compoundsfor biological screening, diethanolamine was treated with isotelekin and isotelekin acetate. A furtherenhancement in rection rate was observed when reaction was done under Microwave Irradiation. Atremendous reduction in reaction time was observed when it took only 5 minutes for the completionof reaction as compared to 4 or 5 hr under normal conditions.Moreover, the yields were higher ascompared to the normal conditions. The structures of all the compounds were elucidated byspectroscopic techniques like IR, ^{1}H NMR, ^{13} C NMR and Mass spectra. All the compounds soobtained were subjected for biological evaluation as plant growth regulators and tested for theirtoxicological behaviour . The parameters studied in biological activity include adventitious rootformation in hypocotyl cuttings of *Vignaradiata*, *Cucumismelo*cotyledon expansion test and seedgermination studies in *Triticumaestivum*. The parameters studied for toxicological behaviour includerecord of mortality, change in diet intake, change in body weight,change in organ weight indices.

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Kinetic investigation of thermal degradation of Cellulose-Reinforced Starch-PVA Blends with insertion of Fly-ash

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Abstract: In the homogenous mixture of Starch and Polyvinyl alcohol (PVA), 30 % of plasticizer was mixed to make Pure blend. Then 10 % cellulose was mixed into above mixture followed by removal of extra water gave Cellulose-Reinforced starch-PVA blends. The different proportions of Fly ash were mixed into mixture of Cellulose-Reinforced starch-PVA blends to get various fly ash inserted Cellulose-Reinforced starch-PVA blends. Thermal degradation of these samples were carried out at various heating rates i.e, 2, 5, 10 and 20 K/min from ambient temperature to 650 ^{o}Cin air. The activation energy for thermal degradation of fly ash blends was more as compare to pure and cellulose-reinforced starch-PVA blends. This conclude that fly ash incorporated blends are more thermally stable than pure or cell blends.

Keywords: PVA, STARCH, FLY ASH, KINETIC STUDIES

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FORMULATION AND EVALUATION OF NANOEMULSION OF FAMOTIDINE

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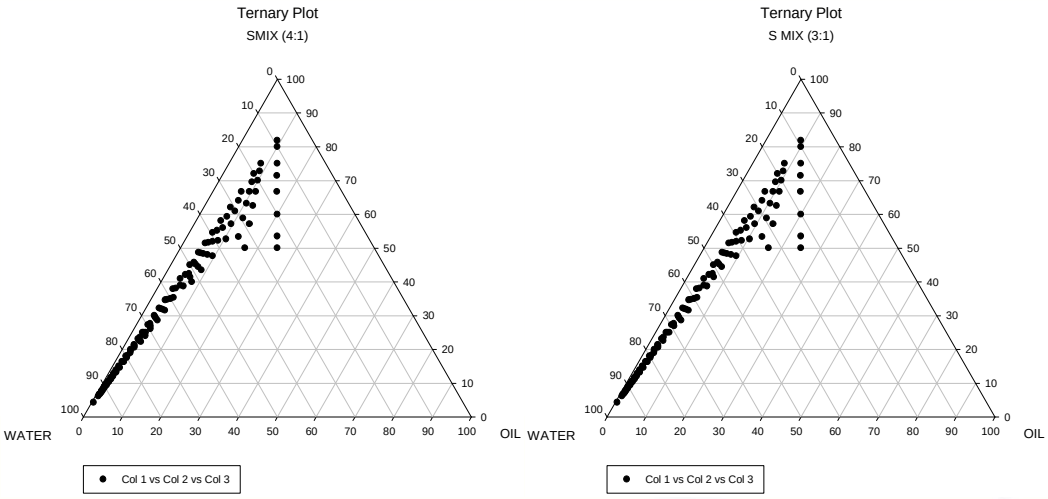
ABSTRACT

Famotidine, a highly lipophilic H_2 antagonist, has poor oral bioavailability (40-45%) due to its low aqueous solubility. Nanoemulsion of famotidine was developed by spontaneous emulsification method with the aim to enhance the therapeutic efficacy of famotidine. Pseudoternary phase diagrams were constructed by aqueous titration technique to identify the nanoemulsion region. Olive oil, Tween 80 and PEG 400 were selected as oil, surfactant and cosurfactant respectively on the basis of solubility study, HLB value and non-toxic nature. The selected formulations from NE region were subjected to droplet size analysis, viscosity study and *in vitro* drug release. The release of drug from nanoemulsion was significantly higher than the pure drug. The optimal formulation containing 6.90% olive oil, 55.16% [Tween 80: PEG 400 (3:1)], and 37.94% by volume of aqueous phase (F2) was selected for *in vivo* study on the basis of higher drug release, lowest globule size, optimum polydispersity value, viscosity and overall lower surfactant concentration and cosurfactant. The *in vivo* studies revealed a significant increase in anti-ulcer activity as compared with standard marketed tablets of famotidine. Thus, nanoemulsions could be used effectively to improve the therapeutic efficacy of poorly water soluble drugs to improve their bioavailability.



Pseudoternary phase diagram of system with the following component:
Oil = Olive oil, Surfactant = Tween 80, cosurfactant = PEG 400

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P-255

Sildenafil and its newly discovered analog compound-4a induced neurodifferentiation in IMR-32 cells

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Abstract: Sildenafil is the first FDA approved PDE5 inhibitor used for the treatment of erectile dysfunction and is currently in research for the treatment of some other diseases also.Treatment of neural progenitor cells with sildenafil has shown to enhance neurogenesis and differentiation by regulation of cGMP levels. cGMP as well as cAMP are known to play a central role in the repair and remodelling of the nervous system during various development stages and in also case of neural injury. In the present study, we reported the neurodifferentiationproperty of sildenafil in an N-mycover expressing neuroblastoma cell line, IMR-32. Sildenafil induces the formation of neurite outgrowths which were found expressing neuronal markers such as NeuN, NF-H and βIII tubulin. A recently discovered sildenafil analogue, compound-4a by our group, which inhibits many PDEs especially PDE5 (IC_{50} 560 nM) and PDE2 (IC_{50} 1.5 nM)more potently than the parent compound, was also found to induce neurodifferentiation of IMR-32 neuroblastoma cells. Both Sildenafil and compound-4a induced the formation of neurite outgrowths, as well as increased the expression of neuronal markers NeuN, NF-H and βIII tubulin in IMR32 cells. Differentiation effect of compound 4a was even more profound than sildenafil. Moreover both sildenafil and compound 4a were found to significantly activate the AMPK-ACC and PI3K-Akt pathways, two important pathways reported to play an essential role in cytoskeletal rearrangements necessary for neurodifferentiation. Our study highlights an idea of repositioning sildenafil and developing compound-4a as lead molecules for the treatment of neuroblastoma.

Keywords: PDE5, Sildenafil, Neuroblastoma, IMR-32, Differentiation, PI3K/Akt,AMPK/ACC

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Diaminomaleonitrile derived efficient ethyl 4-((1Z)-(((1Z)-1,2-dicyano-2-((2-hydroxybenzylidene)amino)vinyl)imino)methyl)-1-phenyl-1H-pyrazole-3-carboxylate: A colorimetric chemosensor for selective sensing of fluoride and acetate ions

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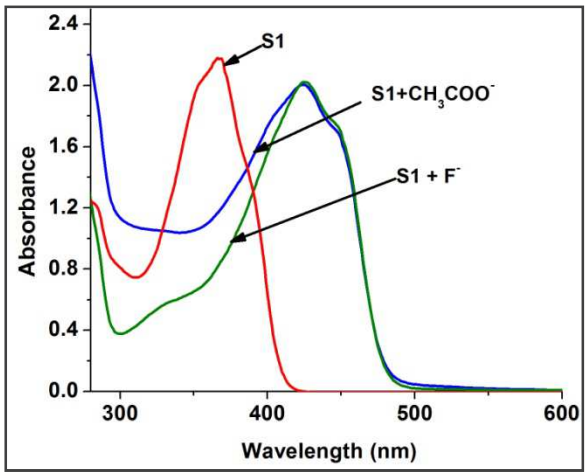
A series of efficient colorimetric chemosensors **(S1-S3)** have been synthesized from 2,3-diaminomaleonitrile, ethyl 4-formyl-1-phenyl-1H-pyrazole-3-carboxylate and 2-hydroxy benzaldehyde. The synthesized sensor molecules were characterized by IR, NMR, mass and UV-Visible spectroscopic techniques. All the synthesized receptors **(S1-S3)** exhibit instant color change from colorless to dark yellow along when interacted with fluoride and acetate ions. The UV-Visible studies revealed that ethyl 4-((1Z)-(((1Z)-1,2-dicyano-2-((2-hydroxybenzylidene)amino)vinyl)imino)methyl)-1-phenyl-1H-pyrazole-3-carboxylate derivatives showed selective sensing towards fluoride and acetate anions in preference to Cl^-, I^-, $H_2PO_4^-$, HSO_4^-, ClO_4^-, Br^- and HSO_4^- ions.



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The Effect of Synthesized Dye on the Electrochemical Behaviour of Copper in 3.5 % NaCl Solution

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Abstract: The facile synthesis of a dye named,4-amino-3-(phenyldiazenyl)benzo[4,5]imidazo[1,2-a]pyrimidin-2(1H)-one,(ABIP) has been done by condensation of 4-aminobenzo[4,5]imidazo[1,2-a]pyrimidin-2(1H)-one and aniline in pyridine. The purpose of this present investigation is to provide a brief mechanistic overview of theelectrochemical behaviour of copper in 3.5% (by weight) NaCl solution by synthesized ABIP. The synthesized dye was characterized by physicochemical analysis. The work has been investigated using potentiodynamic polarization which revealed that the addition of ABIPdecreases current density and consequently increases the corrosion inhibition efficiency of copper in 3.5% (by weight) NaCl solution.

Keywords: Dye, potentiodynamic polarization, Copper, NaCl solution.

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Chemical Investigation of Bombax malabaricum

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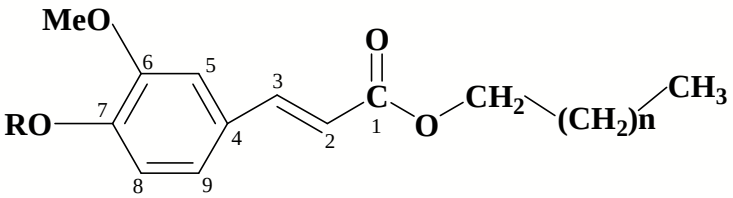
Abstract- *Bombax malabaricum* DC. (syn. *Salmalia malabaricum*), colloquially known as Semul or Red Kapok tree belongs to the family Bombacaceae. Flowers are bitter, acrid, astringent and used as blood purifier.

A hypotensive agent shamimin [1], a C-flavonol glycoside along with mangiferin an antioxidant and analgesic xanthone have been isolated from the leaves of this plant. The xylem of stem, root bark and root exhibited anti-inflammatory and hepatoprotective activity. The methanolic extract of stem bark and lupeol isolated from this extract as a main constituent possess hypotesnive and antiangiogenic activity. The extensive phytochemical examinations of the root, root bark, heartwood and stem bark of this plant have resulted in the isolation of sesquiterpenoids, naphthoquinones, benzopyran dimer shamimicin, steroids and terpenes. The traditional use of the spines of the stem bark as a skin lightener has encouraged us to isolate skin lightening agents from this part of plant. Phytochemical study of this hitherto unexamined part of this species led to the isolation of a new ferulic ester along with known compounds lupeol acetate, stigmasterol, lupeol, friedelin, *trans*-octacosanyl-4-acetoxy-3-methoxycinnamate (**I**) *trans*-triacontanyl-4-acetoxy-3-methoxycinnamate(**II**), *trans*-octacosanyl-4-hydroxy-3-methoxycinnamate(**III**) and *trans*-triacontanyl-4-hydroxy-3-methoxycinnamate(**IV**).



I, R = Ac, n = 26
II, R = Ac, n = 28
III, R = H, n = 26
IV, R = H, n = 28

New ferulic ester **2**, m.p. 85-86^0, was separated as colourless crystals from petroleum ether extract after column chromatography and repeated prep. TLC. The mass spectrum of **2** showed a molecular ion peak $[M]^+$ at m/z 656 which was in agreement with molecular formula $C_{42}H_{72}O_5$.

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P-259

EXTRACTION OF PROTEINS FROM DEFATTED SEED WASTE

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This study presents the extraction of Proteins from defatted seed waste. In our present work we used flaxseed of Indian origin for extraction of oil as well as protein. In initial stages of research we extracted oil from flaxseed which is rich in alpha linolenic acid. After extraction defatted seed cake was utilized for extraction of proteins. Flaxseed cultivated worldwide has attracted people interest for its many human health benefits. Flaxseeds contain about 55 % Alpha linolenic acid (ALA), 28–30 % protein and 35 % fiber. Extraction of proteins was carried out using alkali treatment method. Protein content was estimated using kjeldahl method and amino acid content were analyzed by high performance liquid chromatography method. Glutamic acid (19.2%), Aspartic Acid (9.8%) and Arginine Acid (9.3%) are major amino acids found in the extracted protein powder. This study revealed that amino acid pattern of flax protein is similar to that of soybean protein, which is viewed as one of the most nutritious of the plant proteins.

Keywords: Flaxseed, Protein, Seed Waste, Extraction, Amino acid.

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Quantitation Of Vitamin E in Pharmaceutical Formulation Using Fe(III)/ Fe (II) Redox Couple

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Abstract: A noval, rapid and facile procedure is described for the determination of Vitamin E. It involves the reduction of Fe (III) to Fe (II) with vitamin E that results the formation of pink colored complex of reduced Fe (II) with DMG in the presence of pyridine at pH 6.5-7.2. The absorbance of the complex is measured at 512 nm. Beer's law is obeyed in the range 0.1 to 2.6 ug/ml of vitamin E with molar absorptivity of 2.46×10^{4} l mol^{-1} cm^{-1} The various factors which affect the resulting complex are optimized to obtain maximum absorption. The proposed method is satisfactorily utilized for pure as well as various dosage forms of vitamin E in pharmaceutical formulations which contains common reductants by pre-treatment of the samples.

P-261

Spectrophotometric Quantification of Mesalamine in Pure and Pharmaceutical Formulations

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A new, rapid and facile visible spectrophotometric method has been developed for the determination of mesalamine in pure as well as in pharmaceutical dosage forms. Mesalamine has been used for reduction of Fe(III) to Fe(II) and the reduced iron formed the reddish-pink complex with dimethylglyoxime in presence of pyridine which has absorbance maxima 515 nm. The various conditions which affected the complex formation were optimised to obtain maximum absorption of complex formed. Beer's law was obeyed in the concentration range of 0.2-1.6 µg/ml of mesalamine. The molar absorptivity was calculated to be 3.37×10^3 $Lmol^{-1}cm^{-1}$. The proposed method has been validated statistically. In comparison to some of the existing methods, the proposed method is highly precise and accurate for the spectrophotometric determination of mesalamine in pharmaceutical formulations.

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Quantitation of vitamin C in pharmaceutical formulations using 3-Hydroxy-2-aryl-4H-chromen-4-one as spectrophotometric reagent

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Abstract

A noval , rapid and sensitive spectrophotometric method for the quantitation of vitamin C has been developed. It involves the reduction of iron(III) to iron(II) with vitamin C and the formation of brown colored complex by the reaction of iron(III) with 3-Hydroxy-2-aryl-4H-chromen-4-one , followed by the extraction of the complex into chloroform and measuring the absorbance at 405 nm. Under optimum conditions, Beer's law is obeyed up to 2.4 µg ml^{-1} of ascorbic acid having molar absorptivity and Sandell's sensitivity of 5.897 x 10^{5} l mol^{-1} cm^{-1} and 2.986 x 10^{-4} µg cm^{-2} respectively. The method is free from the various interfering substances including sugars, amino acids and other additives. The method is quite useful and allows satisfactory determination of vitamin C in the presence of common ingredients in pharmaceutical formulations.

P-263

ENVIRONMENT FRIENDLY APPROACH FOR PEST CONTROL BY USING BIO-PESTICIDES

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Abstract

An Environment friendly pesticide is Bio-pesticide which is alternative of harmful chemical pesticides. Chemical Pest Control agents are extensively used in all countries of the world but they are regarded as ecologically unacceptable. The Potential Benefits to agriculture and public health programmes through the use of bio-pesticides are considerable. The interest in bio-pesticides is based on the disadvantages associated with chemical pesticides. In India there is a vast potential for Bio-pesticides. The market share of Bio-pesticides is only 2.5% of the total pesticides market. In India there are many easily available plants like neem, garlic, triphala, pinus etc. which can be easily processed and increase the bio-pesticide consumption in India. This paper highlight role of Bio-pesticides in agriculture and potential bio-pesticides available in India.

Key word: - Bio-pesticide, health, agriculture, chemical, Pest control etc.

P-264

Voltammetric Determination of Palladium (II) In Presence of Iridium (III) And Ruthenium (III)

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Abstract

A simple and convenient method is described for the determination of low concentration palladium based on differential pulse polarographic reduction of Pd(II) in presence of ethylenediamine. Linearity of the calibration curve was achieved upto 27 ppm with a limit of determination 0.01 µg/ml. The possible interference of usually present other transition metals was examined and ruled out. The method has been successfully applied for the determination of palladium in industrial waste water samples.

Keywords: Differential pulse polarography, industrial waste water analysis, new method development, palladium.

P-265

A STUDY OF FATTY ACIDS PROFILES OF MEDICAGO SATIVA AND LABLAB PURPUREUS BOTH BELONGING TO FAMILY FABACEAE

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KEYWORD :- Medicago sativa, Lablab purpureus, Fabaceae, Fatty Acids.

ABSTRACT

Medicago sativa also known as lucerne. It is mainly used as animal fodder. It is an N-fixing legume and does not require added N-fertilizers. Its seed oil contains approx. 17.2% Linoleic acid, 34.5% Linolenic , 35% palmitic 15 % Stearic and 28% oleic and 18% other saturated fatty acids. The Lablab purpureus also known as Hyacinth bean. It has a wide range of medicinal applications and also a good source of manure. Its seed oil contains approx. 10% Linoleic , 12.2% linolenic, 2.1% oleic 4.1% palmitic and1.2% Stearic acid. Both these seeds oil have two major PUFA Linoleic and Linolenic acids and they also have high protein content as a conclusion both these plants may have a potential as a fine source of standard food component as they reduces cholesterol level which is helpful in treating cardiac diseases and also may act as a renewable sources in oil seeds crops.

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Synthesis Characterization and Antiproliferative Studies of some Novel Hydroxypyrazoline

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Abstract: The synthesis of new hydroxypyrazoline as potential multiple target inhibitor is discussed. The aim was to identify the key pharmacophores forantiproliferative activity that can be used for drug development. A series of hydroxypyrazolinederivatives**6a-l** were synthesized and characterized byspectral analysis (^{1}H-NMR, ^{13}C-NMR, Mass and FT-IR).The synthesized compounds were screened for antiproliferative activity against MDA-MB231 and HT-29 human cell linesusing MTT assay. Conjugates **6e** and **6l** exhibited a low IC_{50} valueon MDA-MB231andHT-29 cell linesrespectively. Flow cytometric analysis revealed that, **6e** induced cell cycle arrest in **Go/G1** phase in HT-29 cell lines cancer cells lines. Computational interaction studies of **6e** exhibited its capacity of being a plausible CDK2 inhibitor. In addition**6e** was analysed for DNA binding studies. Binding constant **4.06×10^{6} M^{-1}**indicated that the compoundinteracted through the intercalation mode. All the results stacked together indicated good pharmacological properties.

Keywords: Hydroxypyrazoline, Cytotoxicity, Flow cytometry (Go/G1), CDK, DNA binding

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Antinociceptive activity of stems extract of *Passion fruit*

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*Passiflora foetida L (*family:*Passifloraceae)* commonly known as passion fruit is an exotic fast-growing perennial vine occurring in USA and extended to India. Traditionally, the fresh or dried whole plants and their preparations are accepted for medicinal use in European countries for the treatment of nervous anxiety. It shows antispasmodic, sedative, anxiolytic and hypotensive activities. The decoction from the leaves and fruits of this plant is used to treat asthma and hysteria. It is used traditionally in diseases like diarrhea, headache, intestinal tract, throat, ear infections, fever and skin diseases (Kirtikar, Basu). The ethanolic extract of stems was subjected to preliminary phytochemical tests. Phytochemical investigation of the stem of *Passiflora foetida L* yielded a flavonoid-Apigenin from ethyl acetate extract; Kaempferol, from n- butanol extract and Beta-Sitosterol, from petroleum ether extract. Acute toxicity study of ethanolic extract of stems of *Passiflora foetida L* was carried out and extracts were found to be safe up to 2000 mg/kg body weight. Antinociceptive activities of stems of *Passiflora foetida L* was carried out from aqueous and ethanolic extract by tail flick method in rats and acetic acid induced writhing method in mice(Vogel GH,Vogel WH). Results were found to statistically significant ($P<0.05$) when compared to control.

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An efficient and non-catalyzed facile access to diverse ylidenenitriles and its derivatives via aqua mediated knoevenagel condensation

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Abstract

An efficient, simple, eco-friendly and non-catalyzed method reported for the synthesis of ylidenenitrile and its derivatives via knoevenagel condensation from various heterocyclic carboxaldehyde with active methylene compound viz. malononitrile, ethyl 2-cyanoacetate and cyanoacetamide in presence of distilled water at room temperature and/or at 70-80°c temperature. The % yields of obtained products were compared with the different solvent then water is found as best solvent for this reaction to get very good amount of yield and purity within shorter period of time. The synthesized compounds were characterized for spectral analysis like 1^{H}-NMR, ^{13}C-NMR, and IR.

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SIMULTANEOUS ESTIMATION OF SOME ANTI MYCOBACTERIAL AGENTS BY RP-UPLC

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A simple, sensitive and precise RP-UPLC method for estimation of Pyrazinamide, Isoniazid, Ethambutol and Rifampicin has been developed and validated for determination of compounds in commercial tablet dosage form. The compounds were well separated isocratically on a X Bridge 3x50mm, 3.7 µm C_{18} column using a mobile phase consisting of Solution-A which is composed of phosphate buffer of pH 7.5 adjusted with Ortho phosphoric acid and Solution –B Mixture of Methanol and Acetonitrile in a ratio of 85:15 v/v. Mobile phase used is a mixture of solution - A and solution - B in the ratio of 90:10 v/v. The flow rate was 0.5 ml/min with PDA detector. Retention time for Pyrazinamide, Isoniazid, Ethambutol and Rifampicin was found to be 2.012, 3.120, 4.026, 5.926 min respectively. After suitable dilutions the linear response in the range of 18.75-93.75, 7.5 – 37.5, 20-100 and 11.25-56.25 µg/ml concentration for the Pyrazinamide, Isoniazid, Ethambutol and Rifampicin respectively.Correlation coefficient was found to be 0.999 and slope was calculated. Procedure was extended to formulation of Pyrazinamide, Isoniazid, Ethambutol and Rifampicin, the combination was available in the market of strength Pyrazinamide 750 mg, Isoniazid 300 mg, Ethambutol 800 mg and Rifampicin 450 mg respectively. The precision of the method was determined by % RSD which was less than 1 for all the 4 compounds.

The method was validated in accordance with ICH guidelines. The study showed that the reverse phased liquid chromatography was sensitive and selective for detecting Pyrazinamide, Isoniazid, Ethambutol and Rifampicin using the single mobile phase.

Key words: RP-UPLC, pyrazinamide, INH, ethambutol,rifampicin

P-270

Plant Mediated Bio Synthesis of Silver Nanoparticles: Charecterization and Antibacterial activity

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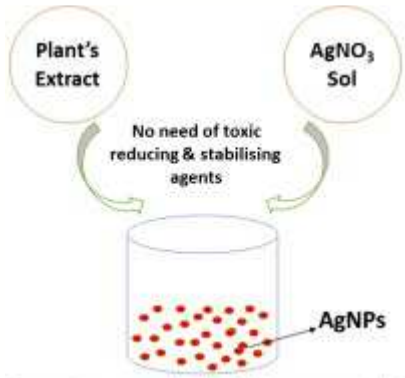
Abstract:- The silver nanoparticles (AgNPs) have gained attraction since last decade and widely accepted in nanotechnology, biotechnology and medicine. The green synthesis of silver nanoparticles has been known for last few years and having their beneficial result. This approach is ecofriendly and less hazardous as compared with other conventional methods. In the light of this, here we reported the synthesis of (AgNPs) by aqueous extract of leafs of variety of medicinally important plant belonging from family *cupressaceae* . During the study multiple changed was observed for different part of different plants, an intense surface resonance Plasmon band in the UV-visible region at 465 nm. The further study of formation of AgNPs were confirmed by FTIR, SEM, TEM and XRD.

Key words : Green Synthesis, Thuja oriental extract ,silver nano particles.



One pot green synthesis of silver nanoparticles

References:-

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INFLUENCE OF STUDENTS' TEST ANXIETY ON SCIENCE ACHIEVEMENTS IN SENIOR SECONDARY SCHOOLS IN AWKA SOUTH LOCAL GOVERNMENT OF ANAMBRA STATE.

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ABSTRACT

This study investigated the influence of students' test anxiety on science achievements in senior secondary schools in Awka South Local Government of Anambra State. Theoretical reports about the adverse effects of test anxiety on science achievement have been rife, but empirical evidence for indigenous samples is necessary. The study adopted the descriptive survey researchdesign. Stratified random sampling was used to selecta sample of one hundred and fiftymales andone hundred and eighty two females' senior secondary school students from the eighteen public secondary schools in Awka South Local Government Area of Anambra State. Five research questions and five null hypotheses were formulated for the study. The main source of data collection was primary data which was collected using Test Anxiety Assessment Scale (TAAS), Biology Achievement Test (BAT), Chemistry Achievement Test (CAT) and Mathematics Achievement Test (MAT). The data collected were analysed using mean, standard deviation, two-way analysis of variance and Pearson momentum correlation. The findings of the study showed a gender difference in test anxiety level and science achievements of the students. Pearson momentum correlation showed an inverse relationship between test anxiety and achievements in science subjects. Male students reported higher test anxiety scores in biology while female students reported higher test anxiety scores in chemistry and mathematics. In contrast, female students reported higher achievement in biology while male students reported higher achievement in chemistry and mathematics. Generally, test anxiety score of the students was highest in mathematics while the achievement score was highest in biology. Also, female students reported higher test anxiety level while male students reported higher science achievement. Analysis of variance showed a significant difference in the test anxiety level and science achievements of the students between gender and subjects ($p<0.05$). There was however no interaction between gender and subject on test anxiety level and on science achievements.This study thus confirms that student test anxiety has a negative influence on science achievement in secondary schools in Awka South Local Government Area of Anambra State. Hence, relevant test anxiety reduction interventions should be adopted by teachers and administrators in secondary schools.

Key words: *students' test anxiety, science achievements, senior secondary schools*

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Synthesis and DNA photo cleavage activities of lanthanum complexes of 4-hydroxy-3-((4-hydroxy-2-oxo-2H-chromen-3-yl)(3-(4-nitrophenyl)-1-phenyl-1H-pyrazol-4-yl)methyl)-2H-chromen-2-one and 4-hydroxy-3-((4-hydroxy-2-oxo-2H-chromen-3-yl)(1-phenyl-3-p-tolyl-1H-pyrazol-4-yl)methyl)-2H-chromen-2-one

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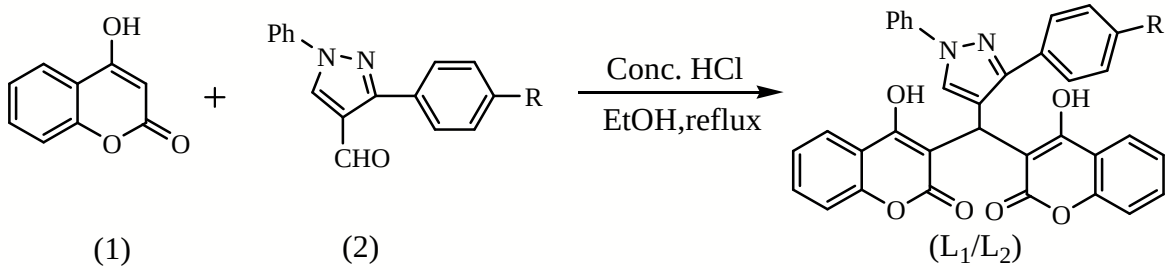
Coumarins and their complexes seeks the attention of researchers due to their enriched biological and pharmaceutical profile. The complexation of transition metals with ligand is reported with biological activities such as antitumor, anti-inflammatory, anti-parasitic properties, as well as uses against other diseases. On the other side, the chemistry of lanthanides is well known to us. But their complexes are not widely explored in the literature. Some reports revealed that complexes of lanthanides are associated with a number of biological properties such as cytotoxic effect and anticancer effect. By taking this into consideration, we have integrated the biscoumarins, as ligand and lanthanum. The ligands (L_1 and L_2) were generated by refluxing the ethanolic solution of 4-hydroxycoumarin and 1,3-diphenyl-1H-pyrazole-4-carbaldehyde (2) for 25 minutes in presence of HCl.(Scheme 1)



(1) (2) (L_1/L_2)

The ligands were subjected to the lanthanum nitrate hexahydrate to show the complexation ability of these ligands with lanthanum(III) ion. Furthermore, we have taken the consideration of DNA photo cleavage activity of synthesized complexes. From overall results, it is evident that complexes 1 and 2 can be recognized as the most biologically active members of this study and can be used as DNA photo cleaving agents in future.

Keywords: Courmarin, lanthanum complexes, DNA photocleavage.

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Design and Synthesis of novel 4-{[(5*Z*)-5-(1*H*-indol-3-ylmethylidene)-4-oxo-4,5-dihydro-1,3-thiazol-2-yl]amino}benzenesulfonamide as potent inhibitor of Zika Virus NS3 helicase

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In the present study, we have focused on the design and synthesis of thiazolidinone derivative for potent inhibitor of Zika Virus NS3 Helicase. Initially 4-[(4-oxo-4,5-dihydro-1,3-thiazol-2-yl)amino]benzenesulfonamide is synthesized, which is then converted into 4-{[(5*Z*)-5-(1*H*-indol-3-ylmethylidene)-4-oxo-4,5-dihydro-1,3-thiazol-2-yl]amino}benzenesulfonamide by refluxing indole-3-carboxaldehyde in the presence of piperidine in 1,4-dioxane. The compound is characterized by FTIR, ^{1}H-NMR, ^{13}C-NMR, LC-MS spectroscopy. The compound is docked to ATPase active site of NS3 helicase isolated from Zika virus. The compound has shown strong binding affinity at ATPase site with dock score -9.111 and binding energy -59.267.

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Facile and effective approach for oxidation of boronic acids

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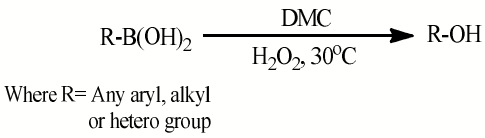
Abstract

This present work illustrates facile and effective approach for oxidation of boronic acids using environmentally benign dimethyl carbonate (DMC) as a solvent with H_2O_2 as an oxidant at room temperature. In contrast to previous reaction reports, which make use of metal catalyst, hazardous reagent and oxidants that creates environmental concern. This method provides good to excellent yield of products and showed better tolerance towards various functional groups present on boronic acids. Moreover, this developed process is an alternative in terms of inexpensive, non toxic and easy reaction conditions.

General Scheme



Where R= Any aryl, alkyl or hetero group

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IMPROVED SYNTHESIS OF MEDIUM CHAIN TRIACYLGLYCEROL BASED ON USE OF SUPERCRITICAL CARBON DIOXIDE PRETREATMENT

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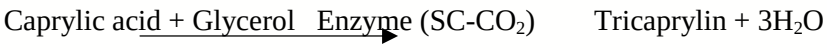
Abstract

The esterification reaction of glycerol and caprylic acid catalyzed by immobilized lipase in the presence of supercritical carbon dioxide has been investigated in the present work also quantifying the intensification benefits. Factors influencing the progress of enzymatic reaction in term of the pretreatment conditions, reaction time, reaction temperature, molar ratio of substrate, enzyme loading and type of enzyme, were varied to establish the effect on the progress of reaction. Optimum conditions for pretreatment using supercritical CO_2 were established as time of 1h, pressure of 100 bars and temperature of 50^{o}C. Use of pretreatment resulted in a conversion of free fatty acids to tricaprylin as 97.3% in 6h of reaction time at 50°C and molar ratio of 4:1(Caprylic acid: glycerol) under optimized reaction conditions. It was established that pretreatment resulted in three times higher yield as compared to conventional approach. Two immobilized biocatalyst as Novozym 435and Lipozyme RM were used and it was established that Novozym 435 showed better catalytic activity as compared to Lipozyme RM, though importantly both were active even in the presence of supercritical carbon dioxide. Overall, it has been established that use of supercritical carbon dioxide for pretreatment was more efficient and enhanced the rate of synthesis of tricaprylin as compared to conventional approach.

General Scheme



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P-276

Straightforward synthesis and catalytic applications of rigid N,O-type calixarene ligands

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Unlike more popular ligand systems that contain a combination of hard and soft heteroatoms, calixarene molecules possess only phenol-based hard donor centers which impair their coordination properties and catalytic behavior. To address this issue, we earlier reported the first N,O-type calixarene ligand 2 (Scheme 1, previous work) where two of the phenol groups were re-placed with soft triazole rings. Here, we report a simple one-step access to new rigid N,O-calixarene ligands which is based on copper-catalyzed amination at the lower rim. We also present coordination properties of these ligands with some main group and transition metals leading to new complexes with superior catalytic activity, in several organic transformations, compared with calixarene metal complexes reported in the literature.

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P-277

Inhibition of H3K9 methyltransferase G9a repressed cell proliferation and induced autophagy in MCF-7 cells

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Keywords: Posttranslational modifications,Methyltransferase,G9a, autophagy,cancer and genome organization.

Posttranslational modifications of histones are important in maintaining and regulating genome organization. These modifications include Acetylation, Methylation, Sumolyation and Ubiqutination.These modifications usually occur at lysine residues. Any aberration in these modifications can lead to serious diseaseslike cancer due to change in 3D genome organization. Targeting of methyltransferases by inhibitors has proved useful for controlling various abnormal states resulting from aberrant methylations. This study was carried out to find an inhibitor against G9a, a methyltransferase.Institutional natural product library comprising 600 compounds was screened by using Enzyme based assay.Seven hits were identifiedand their IC_{50} was determined, ranging from 0.4-8µM. Among them, one inhibitor,COD18B with IC50 of 2.04µM,impairs the G9a HMTase activity resulting in the reduction of H3K9me2 in cell based assays.Moreover, we showed that inhibition of G9a leads G2/M arrest and autophagy-associated cell death using FACS and western blottingrespectively. Together, these results suggest that COD18Binduces autophagy-dependent cell death via G9a dysfunction in MCF-7 cells.Therefore G9a inhibition can be an effective therapeutic strategy for cancer treatment.

P-278

Glycemic Index of *Caryota urens* (Kithul) Treacle and Jaggery; Traditional Natural Sweeteners of Sri Lanka

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*Caryota urens (*Kithul), is one of the native sugar palms in Sri Lanka. Traditionally, young inflorescence of *C. urens* is tapped for its sweet phloem sap, which is used to produce sweeteners (treacle & jaggery) and fermented beverage (toddy). It is shown to possess several medicinal properties such as antioxidant, anti-diabetic [1,2]. The objective of this study was to determine the glycemic index of two commonly used traditional sweeteners in Sri Lanka; kithul treacle and jaggery. A randomized clinical trial was carried out according to WHO/FAO guidelines [3]. After overnight fasting, eleven healthy volunteers consumed treacle, jaggery and glucose (as the reference) containing 50 g of available carbohydrates on different days with a minimum gap of 7 days. The reference was repeated two times on each subject in between test foods with a minimum gap of seven days. Blood glucose levels were assessed at time points of 0 (before consumption), 15, 30, 45, 60, 90 and 120 minutes after. Incremental area under two-hour blood glucose response for each person was used to calculate GI. The mean age of the participants was 26.8 ± 4.96 years (range: 20–36 years), mean body mass index (BMI) of 24.94 ± 5.2 kg/m^2(range: 17.6 – 33.3), and mean HbA1c% was 5.27 (range: 4.9–6). GI values were found to be 27.84 for treacle and 31.34 for jaggery. Our results indicate low GI values and, therefore kithul treacle and jaggery can be recommended for diets of diabetic patients as a superior substitute for white sugar.

Keywords—Glycemic index, *Caryota urens*, natural sweeteners, diabetes

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P-279

Carbondot based fluorescence sensor for retinoic acid

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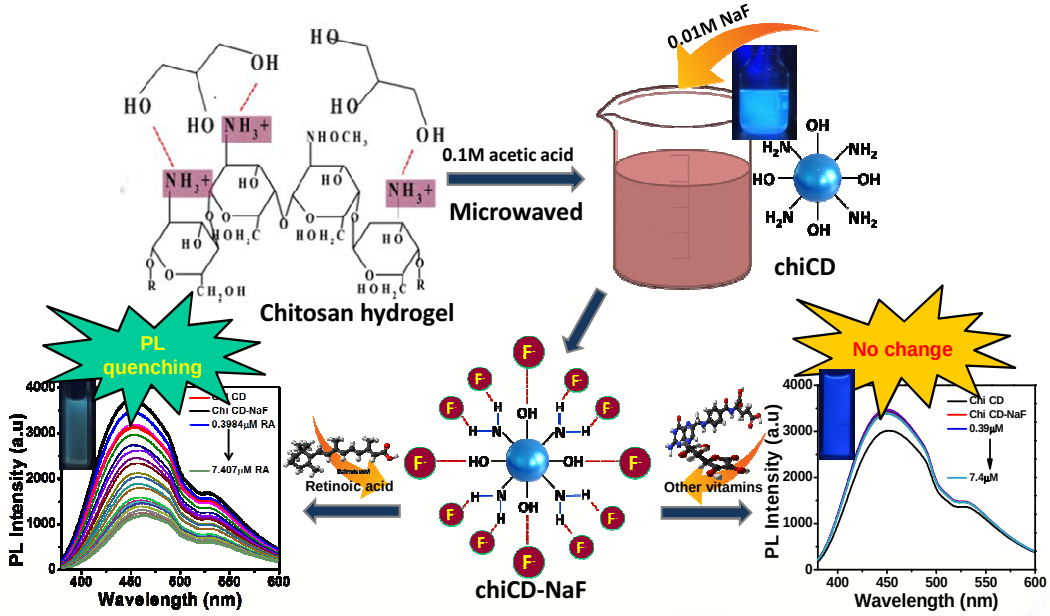
Abstract: In this work chitosan carbon dot (chiCD) based fluorescence sensor was developed which can selectively detect Retinoic acid (RA). The CDs were prepared from chitosan hydrogel and further conjugated with NaF to develop a chiCD-NaF system for the detection of Retinoic acid based on its PL properties. It was found that addition of NaF resulted in the enhancement of fluorescent spectra of chiCD. Addition of RA to the chiCD-NaF system resulted in quenching of the PL spectra. The detection of RA was selective as there is no change in PL properties using other vitamins viz. Ascorbic acid, Choelcalciferol, Folic acid, Riboflavin, Tocopherol etc. The chiCD-NaF systems were also checked with two commercially available capsule containing mixtures of vitamins and here too PL change was insignificant demonstrating selectivity of RA. A probable mechanistic behaviour of the system towards different vitamins is also explained in this paper.



Scheme1: Schematic representation of procedure adopted in fabricating a fluorescent based sensor for Retinoic acid.

P-280

Design and development of novel hydantoin derivatives as androgen receptor antagonists

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Abstract: Prostate Cancer (PCa) is one of the most frequently diagnosed noncutaneous tumour worldwide. Androgen receptor (AR) is a DNA-binding transcription factor, belonging to the nuclear receptor subfamily and is a key signalling pathway leading to the emergence of PCa. Since 2010, Abiraterone acetate, Cabazitaxel, Docetaxel plus prednisone, enzalutamide and sipuleucel-T have been approved by U.S. FDA for the treatment of patients with castration resistance prostate cancer (CRPC).1 The treatment of CRPC is challenging due to AR overexpression and mutations. Furthermore, CRPC expresses the cytochrome P450 enzymes for intratumoral androgen production. In a previous study, we have reported the design and synthesis of several oxobenzimidazoles and thiazolidinediones that demonstrated the relevant cytotoxicity and pharmacokinetic properties.2 Hydantoin derivatives possess a wide diversity of important biochemical effects and interesting pharmacological properties.3,4 In particular, spirohydantoin derivatives represent a potential starting point in discovering new and potent antitumor agents with cytotoxic activity on ovarian and breast cancer. More recently, hydantoin derived guanine oxidation products have emerged as markers of oxidative cell damage. These hydantoins are significant DNA lesions that are targeted by repair enzymes and may be implicated in cancer, aging, and neurological disorders. In this study, we employed the experimental and computational methods to investigate the interference of hydantoin derivatives with the androgen receptor against prostate cancer. Interestingly, compounds like MDV 3100, ARN-509, ONC1-13B, bind to the AR with high affinity and demonstrated strong antagonist activity in the prostate, which seemed to be more potent than bicalutamide. However, nearly it will become resistance to the PCa patients. In addition, AR gene mutation, such as T877A and W741C/L and bone metastasis remain the major challenges for the clinical management of this cancer. Prior to undertaking synthesis, *in silico* molecular docking was performed to understand the binding mode of our hydantoin analogues. Based on the molecular docking results, the synthesis of NCEs was carried out by the conventional methods through isocyanate intermediates (Fig. 1).

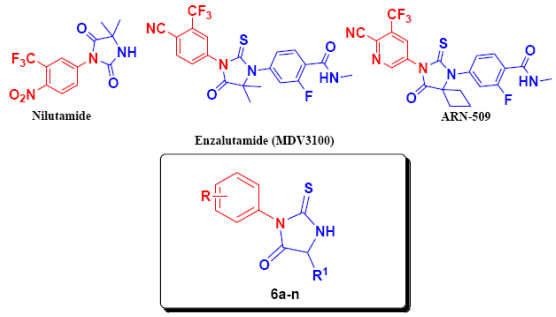

Fig. (1). Structural modification of novel designed hydantoin derivatives

The NCEs was evaluated by using MTT assay. Further, the mechanism of action will be studied by measuring transcriptional proteins using RT-PCR or Western blot analysis, Plasmid and siRNA transfection assay, Immunohistochemical analysis. Finally, the best molecules will be taken for PCa in vivo xenograft model.

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P-281

DESIGN AND SYNTHESIS OF NOVEL SELECTIVE SEROTONIN REUPTAKE INHIBITORS AS POTENTIAL ANTIDEPRESSANT AGENTS

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ABSTRACT

Depression is a significant contributor to the global burden of disease and affects people in all communities across the world. Today, depression is estimated to affect 350 million people. The World Mental Health Survey conducted in 17 countries found that on average about 1 in 20 people reported having an episode of depression in the previous year. [1] During the past two decades, selective serotonin reuptake inhibitors (SSRIs) have been proved to be a safer and more effective resistance than the first-generation antidepressants (TCAs and MAOIs).[2] The research present herein focused on the design and synthesis of novel series of SSRIs by taking a Fluoxetine as a reference molecule. Novel chromane moiety with different substituents at 4th position is the structural scaffold of present study. Series of chromane derivatives have been synthesized having substituted piperazine side chain. Compounds were characterized by IR, ^{1}H NMR, ^{13}C NMR and Mass spectra. All the synthesized compounds were found to promising antidepressant activity. Among the series two compounds were found to more active than standard Fluoxetine in tail suspension test (TST). [3] These two compounds were evaluated for serotonin reuptake inhibitor activity by 5-HTP potentiating test [4] in mice and both the compounds were found to selective serotonin reuptake inhibitors and highly selective toward serotonin transporter. This new structural scaffold (Chromane) with piperazine side chain may open new era of antidepressant agents with selective serotonin reuptake inhibitor activity.

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P-282

DEVELOPMENT OF POLYVINYLALCOHOL FORMALDEHYDE COMPOSITE FOR ELECTRICAL SENSING OF ACETONE VAPOR

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The synthesis, characterization and development of a selective electrical sensor of Acetone from conducting polymer (PFG) based on Polyvinylalcohol is reported here. The synthetic route followed a simple one pot approach of thermal polymerization method using PVA, formaldehyde and glycerol. P. Dutta et. al. [1] synthesized ammonia sensor via a similar technique using methacrylic acid and glycerol. The compound PFG was characterized using FTIR, TGA, DSC, AC Conductivity and FESEM. In this study, the alternating current conductivity measurementswere carried out within the temperature range of 30–90◦C and the frequency range of 1 Hz–100 kHz insolid state. Complete electrical studies including impedance, dielectric, ac conductivity, current−voltage andtransport number measurements were carried out and showed significant results. B. Gogoi et. al. [2] carried out the impedimetric sensing of Picric acid using the same technique of LCR. A three-fold decrease in conductivity was observed upon exposure to acetone vapour. Acetone was taken as the analyte after studying the “diabetic ketoacidosis”. Our finding demonstrates for the first time theac electrical impedance based Acetone detection using polymeric composite.The ionic transport number was measured with thehelp of the Wagner polarization technique. The circuit design is given as Fig A. The experimental setup is demonstrated in Fig. B.

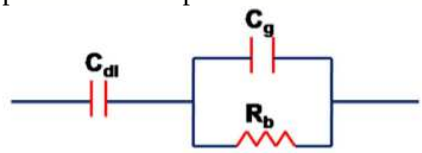

Fig. A

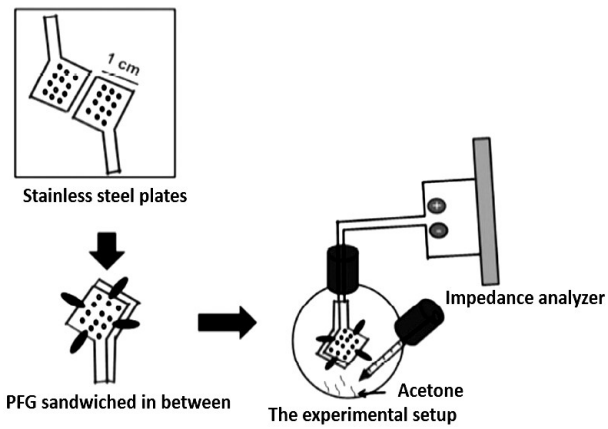

Fig. B

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P-283

Nanocurcumin and polyvinyl alcohol doped nanocurcumin: Synthesis, properties and anti-microbial activity

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Curcumin is widely used as therapeutic and anti microbial agent. Here we have synthesised curcumin nanoparticle using a simple technique(1). The nanoparticles were characterised using zeta-sizer confirming the formation of nanoparticles. The same has also been confirmed using FESEM and AFM. The nanoparticles were doped with polyvinyl alcohol (PVA) to develop a PVA-CurN film. This nano-composite was characterised by FT-IR, UV-Vis, AFM, TGA, DSC, XRD spectroscopic techniques. The electrical properties were also investigated. Curcumin, which is a well known anti-microbial agent, when doped with a bio-compatible polymer, PVA gives a non-toxic and biodegradable biopolymer. Study on the anti-microbial activity of this film was carried out, and this makes the PVA-CurN film a potential candidate as a wound dressing material.

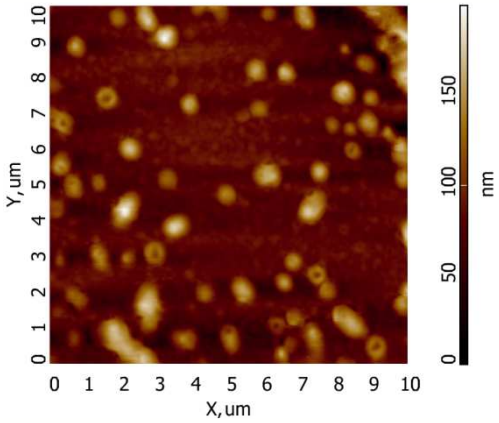

Fig.1: AFM image

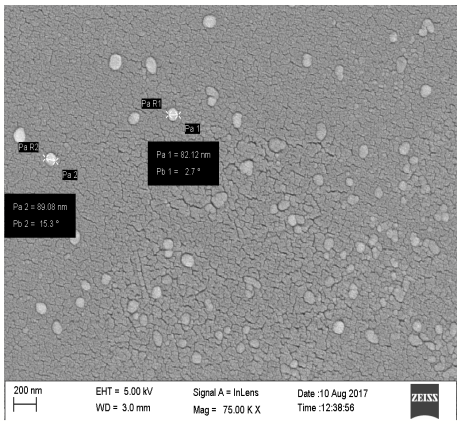

Fig.2: FESEM image

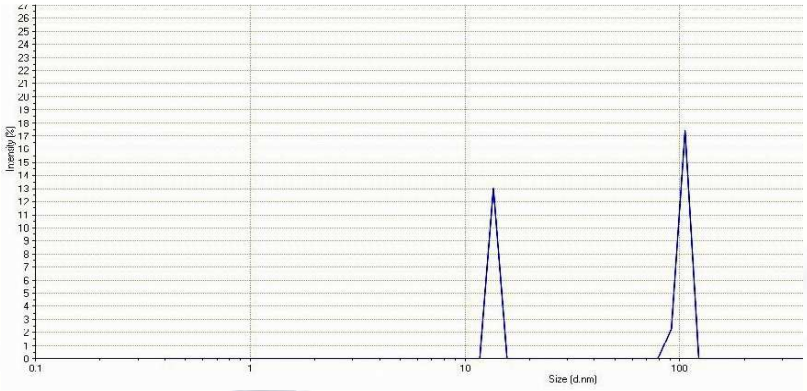

Fig.3: Zeta Sizer

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P-284

New types of n-type organic semiconductors based on Dithioketopyrrolopyrroles and Benzochalcogenadiazoles: A DFT study

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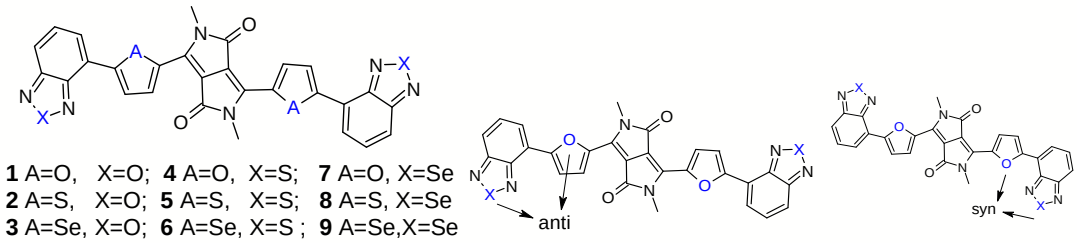
The relatively less number of n-type organic semiconductors (OSCs) or electron transporting molecules as compared with the hole transporting molecules is due to the instability of the anion (formed by accepting electron in n-type OSCs) in air as these tend to react with O_2 and H_2O. So, there has been recent thrust in the design of new types of n-type compounds. Various moieties that have been extensively employed for the synthesis of n-type semiconductors include dithioketopyrrolopyrrole, benzochalcogenadiazole, naphthalene tetracarboxylic dianhydride, perylene tetracarboxylic dianhydride etc. Our present study involves computational studies on the combination of two or more known acceptor moieties, in particular the dithioketopyrrolopyrrole (DPP) and benzochalcogenadiazole (BTz) moieties to get new class of n-type OSCs. Altogether nine model compounds (**1**-**9**, Fig 1a) have been designed and investigated computationally for their n-type properties at B3LYP/6-31G* level. These model compounds were found to possess low electron reorganization energies (0.14-0.18 eV) as compared with their hole reorganization energies (0.24-0.25 eV). The charge mobilities calculated according to the dimer model (at a distance of 4 Å between the dimers) showed that they possess relatively higher electron mobilities (2.9-7.4 cm^2/Vs) with their hole mobilities being in the range of 0.86-1.56 cm^2/Vs and thus points their suitability as ambipolar n-type organic semiconductors.



1 A=O, X=O; **4** A=O, X=S; **7** A=O, X=Se
2 A=S, X=O; **5** A=S, X=S; **8** A=S, X=Se
3 A=Se, X=O; **6** A=Se, X=S ; **9** A=Se,X=Se

(a) (b) (c)

Fig 1: (a) Structures of the studied model compounds of BTz-DPP-BTz type and (b) their *anti* and (c) syn conformation.

P-285

Synthesis, Spectroscopic and ultrasonic studies of Cu (II) surfactant derived from Karanj *(Pongamia pinnata)* oil in methanol-benzene mixture.

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Abstract

Synthesis of Cu (II) soaps derived from non - edible oil i.e. Karanj and its complex with 2-amino-6–methyl Benzothiazole for comparative studies. Spectral studies (IR and NMR) have been carried out to understand the structural insight of the soaps and complex synthesized [1]. Micellar characterization of Cu (II) soaps derived from Karanj Oil has been looked into using benzene and benzene –methanol (two compositions) as the solvent [2-3]. Ultrasonic interferometer, one of the versatile techniques, was used to study the binary and ternary systems. Ultrasonic speed have been measured in binary and ternary systems containing Copper soap derived from Neem oil in 100% benzene, 80 % and 60% methanol benzene mixture. From these values, the specific acoustic impedance Z, adiabatic compressibility β_{ad}, intermolecular free length L_f, apparent molar compressibility $_k$, molar sound velocity R, primary solvation number $S_n$have been calculated. The results have been fitted to Bachem's and Masson equation.

Key words: Cu (II) Soap, Non-edible oils, Soap- Solvent interaction, CMC, Ultrasonic.

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P-286

One Pot Synthesis and Characterizations of Polyfunctionalized Pyrimidine for the Development of Novel Leads for their Biological Potency

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Nitrogen containing heterocycles are important class of compounds as they have proved promising role as potential pharmacophores. Among these heterocycles containing pyrimidines moiety have been shown to possess wide range of biological activities [1-3] such as 5-fluorouracil as anticancer; idoxuridine and trifluoridine as antiviral; zidovudine and stavudine as antiHIV; trimethoprim, sulphamethiazine and sulphadiazine as antibacterial; sulphadoxin as antimalarial and antibacterial; minoxidil and prazosin as antihypertensive; barbiturates eg. phenobarbitone as sedative, hypnotics and anticonvulsant; propylthiouracil as antithyroid; thionzylamine as H1-antihistamine; and toxoflavin and fervennuline as antibiotics. The presence of a pyrimidine base in thymine, cytosine and uracil, which are the essential binding blocks of nucleic acids, is one possible reason for their activity. Keeping in view importance of nitrogen heterocycles in antiparasitic area and our continuous effort to search the novel bioactive nitrogen heterocycles, recently, we have designed the one pot synthesis of poly functionalized for the development of novel leads for their biological potency. In this presentation, the detailed synthetic procedure, mechanisms of the reactions and characterizations of the synthesized compounds by their spectral data (^{1}H NMR, ^{13}C NMR, EIMS, UV and IR) analysis will be discussed.

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P-287

A facile synthesis and determination of their inhibition properties against *β*-lactamase enzyme of some novel tetrazole containing maleamic acid, maleimide and isomalimide derivatives.

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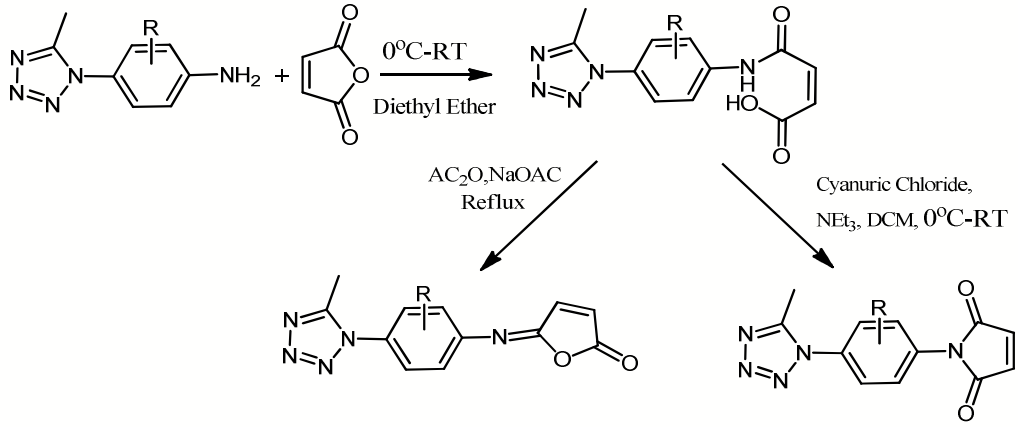
Abstract: Different maleamic acid, maleimide and isomalimide derivatives are the most extensive class of organic chemistry useful in applications such as biological and pharmacological activities. Tetrazole containing maleamic acid, maleimide and isomalimide derivatives shows inhibition properties against *β*-lactamase enzyme, antibacterial, antifungal activities.



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P-288

Anti-allergic

Neel k patel, jaimin b patel, Tarun m. Patel

Kadisarva vishwavidyalaya

Abstract:

Agents that are used to treat allergic reactions. Most of these drugs act by preventing the release of inflammatory mediators or inhibiting the actions of released mediators on their target cell. Several types of allergy treatments are available-allergy shots, antihistamines, cromolyn, leukotriene blockers, and nasal steroid sprays. This report focuses on second generation Anti-histamine pills and nasal sprays, such as allegra, clarinex, Claritin, xyzal and Zyrtec.

P-289

Multicomponent Synthesis of Aryl Substituted 3-(4,6-dichloro-1,3,5-triazin-2-yl)thiazolidin-4-ones and Evaluation of Their Biological activity

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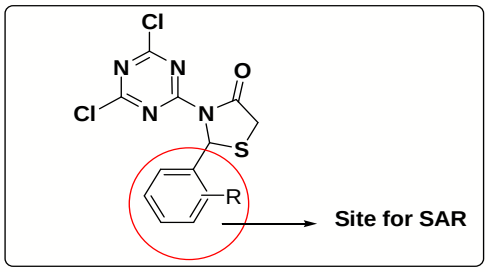
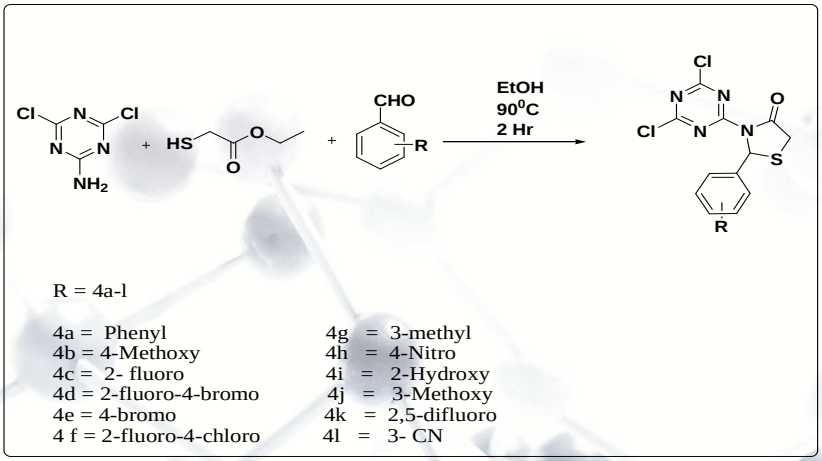
ABSTRACT: A frequent approach to synthesize a series of 3-(4,6-dichloro-1,3,5-triazin-2-yl)-2-phenylthiazolidin-4-one was developed by applying an efficient multi-componant reaction. Also, the synthesized compounds were tested for their antimicrobial activity. The most admirable results were observed with the substituted phenyl thiazolidin-4-one triazine analogs and it could be a potential starting point to develop innovative lead compounds fight against a panel of some human disease-causing pathogens bacteria and fungi. All synthesized compounds were characterized by IR, ^{1}H NMR, mass and elemental analysis.



Our synthetic strategy for novel compounds was outlined in Scheme 1. The synthesis of thiazolidinone triazine derivatives was achieved by the reaction between aromatic aldehyde was condensed with triazine amines and ethyl 2-mercaptoacetate using ethanol, which were cyclized to form final thiazolidinone derivatives. The accuracy of the synthesis of compounds was confirmed on the basis of ^{1}H NMR, Mass spectra and elemental analysis. All newly synthesized compounds were subjected to anti-microbial activity against various gram-positive, gram-negative bacteria and fungal strains by using an agar well diffusion method. [2] The antimicrobial activity of these compounds to further assist for SAR study. The final compounds were screened against a panel of human disease-causing pathogens consisting of four gram-positive and four gram-negative strains as well as antifungal strain.

Keywords: Synthesis, Characterization, Thiazolidinone , Antibacterial, Antifungal activity, s-Triazine .



Scheme-1: Synthesis of 3-(4,6-dichloro-1,3,5-triazin-2-yl)-2-substituted phenylthiazolidin-4-one:

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P-290

Synthesis, Characterization and Biological studies of Novel Pyrazole Derivatives

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The research to obtain new antibacterial compounds is important. Recently due to improper and excessive use of antibiotics, there has been an increasing rate antibiotic resistance in bacterial strains. Thus new compounds bearing rhodanaine and derivatives which may be useful as antibacterial agents have been examined. In an attempt to synthesize the new bioactive heterocyclic analogs, a series of novel pyrazole derivatives featuring rhodanine, its derivatives and analogs were synthesized and characterized by ^{1}H-NMR, ^{13}C-NMR, FT-IR and ESI-MS techniques. These compounds were also evaluated for antibacterial studies using gram positive and gram negative strains. This work will be presented on "**24th ISCB International conference (ISCBC-2018)"at Manipal University Jaipur, India.**

P-291

SYNTHESIS OF SUPRAMOLECULAR SENSORS TO DETECT AMINO ACIDS

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Amine compounds as one of the common organic compoundsin the world are very important in biology system [1]. In therecent years, amine compounds seem to fascinate a lot of scientists,because the amine compounds can form very important biologicalsubstances like amino acids, neurotransmitters, enzymes, etc[2].Apparently, the disorder states of these biological substances maylead to very serious problems for human body. For example, thelacking of amino acids like Histidine (His) and cysteine (Cys) maylead to a series of metabolic and heart diseases like Alzheimer'sdisease and coronary heart disease [3].Thus, it is of great importance to design anddevelop sensors to detect all kinds of amine compounds selectivelyand sensitively.

Resorcinarene molecule have eight hydroxyl group at upper rim of the molecule where substitute any other functional group. Between the two hydroxyl group one hydrogen present where many functional group are introduced like sulphonic acid, halides, hydroxyl, carboxylic acid, methyl halides, etc. To introduce formyl group at this position, it is necessary to investigate a method which is time saving, ecological, economical and higher yield.

The supramolecular sensor was designed and synthesized for the detection of different amino acids. Thissensor with formylatedresorcinarene structure was achieved by the reaction of resorcinarenethrough Duff reaction.The fromyl groups are attached to upper rim carbon between two hydroxyl groups. The target molecules were purified by column chromatography and characterized by NMR, IR and ESI mass spectra. By introduction of formyl group at upper rim, we extended the functionality of Resorcinarene, and they can be used as sensor for various amino acids.

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P-292

Exsolution of Metal Catalysts for Dry Reforming of Methane

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Abstract: Dry reforming of methane (DRM) has received considerable attention in recent years. A major limitation of DRM is catalyst deactivation either by sintering, unwanted oxidation or carbon accumulation on active sites of the catalysts. The development of tailored functional materials consists of active metal catalysts dispersed on surface play an important role in reforming of methane for synthesis gas production. Mostly, these types of structures were prepared by deposition techniques. Here, we demonstrated active metal catalyst exsolved onto the surface of oxide using perovskite as a supporting network and their potential application for methane dry reforming. We have synthesized shape-control of the parent $LaNiO_3$ Perovskite nanoparticle by chemical routes resulting into cubes, spheres, and rods. The shapes of parent perovskite highly influence the spatial distribution of exsolved Ni crystals on La_2O_3 supports, and provide a strong catalyst-support interaction, lead to coke- and sinter-free catalytic methane oxidation. We found that the catalysts derived from $LaNiO_3$ spheres and rods were free of carbon accumulation after 100 hrs of reforming while those derived from cubes showed excessive carbon accumulation and signs of sintering.

Keywords: Perovskite, shape control, $LaNiO_3$, in-situ, dry methane reforming, alloy

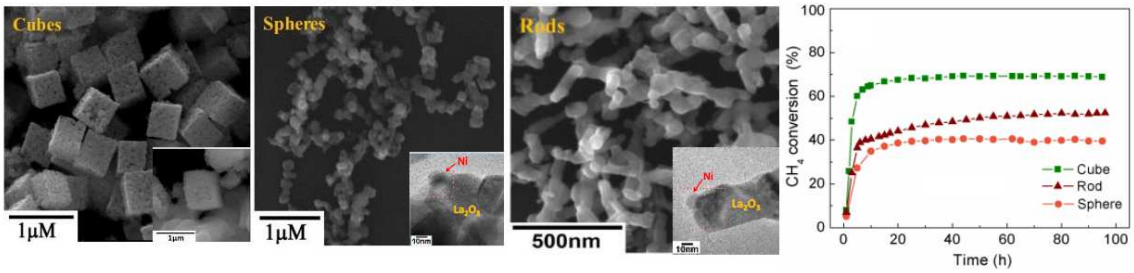

Fig. 1. SEM images of cube, sphere and rod shape perovskite precursor. Inset shows TEM images of their corresponding active catalyst where Ni exsolved on La_2O_3 support after reduction treatment. Last images shows methane conversion after 100 hrs reaction over Ni catalyst derived from cube, sphere and rod shape perovskite.

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P-293

Resorcinarene Stabilized Nanoalloy for SelectiveSensing of Cu(II) ionsin Aqueous Medium bySpectroflourimetry

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Abstract

The newly synthesized Calix[4]resorcinarene tetrahydrazide (CRTH) was characterized by ^{1}H-NMR, ^{13}C-NMR and ESI-MS. It was further used as reducing as well as stabilizing agent for the synthesis of bimetallic nanoparticles (AuAgNPs). The obtained CRTH-BMNps were characterized by Surface Plasmon Resonance (SPR), Particle size analyzer (PSA), Transmission electron microscopy (TEM) and Energy dispersive X-ray (EDX). CRTH- BMNps were probed for their stability at different temperature. Their interaction with various metal ionslike Cr(II), Mn(II), Fe(III), Co(II), Ni(II), Cu(II), Zn(II), Cd(II), Pb(II), Hg(II)was checked by spectrophotometry and spectroflourimetry. The spectra unfolded that CRTH-BMNPsare meticulously selective and sensitive for Cu(II) ions by means of fluorescence quenching. This method allows rapid and accurate determination of Cu(II) ions in aqueous medium at room temperature. The minimum detection limit was found in the range of 1nM to 2.08 µM. The CRTH-BMNPs also behaved as a sensitive nanoprobe for detection of Cu(II) ionsin industrial waste water sample.

P-294

Dependance of mesomorphism on terminal substitution of azoester series

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ABSTRACT

The synthesis of a novel azoester homologous series was carried out with a view to understanding and establishing the effect of molecular structure on liquid crystal behavior of a substance. Transition and melting temperatures, textures of LC were determined by an optical polarizing microscope equipped with a hot stage. The textures of nematic mesophase are schlieren or threaded. Transition curves of a phase diagram behave in a normal manner.The authors have synthesized novel LC compounds, evaluated their LC properties and characterized respective molecular structure of novel LC material. Thus, dependence of mesomorphism and the degree of mesomorphism on the molecular structure are mainly studied by Gray et al. [1-3].Thus, study is aimed to understand and establish the effect of molecular structure on mesomorphism as a consequence of molecular rigidity and flexibility [4-6].

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P-295

A facile one spot synthesis of novel 1*H*-dipyrazolo [1,5-*a*:3',4'-*d*] pyrimidine derivatives

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Abstract:

A facile method one spot synthesis of derivative 1*H*-dipyrazolo [1,5-*a*:3',4'-*d*] pyrimidine (RV1-RV10) were synthesized by the reaction of 3-methyl-1*H*-pyrazol-4(5*H*)-one, substituted aldehydes and 3-phenyl-1*H*-pyrazol-5-amine thermally and microwave mediated reaction. Good yield under microwave condition in ethanol. All the synthesized molecules were characterized by their spectral study IR, MS, ^{1}H and ^{13}C NMR.

P-296

Electrochemical approach for synthesis of 3-substituted indole derivatives

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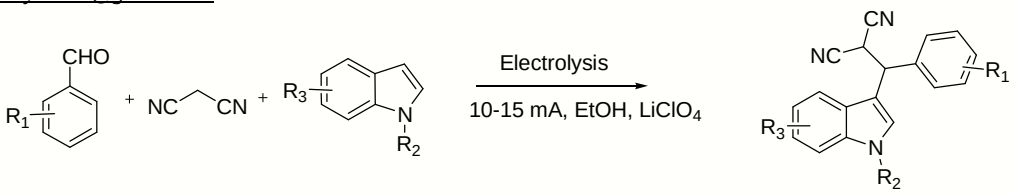

Multi-component reactions (MCRs) are novel synthetic methodologies for the preparation of compound libraries which is pivotal focal point of research activity in the field of modern medicinal and combinatorial chemistry[1]. In recent years, the synthesis of combinatorial small-molecule heterocyclic libraries has emerged as a valuable tool in the search for novel lead structures.[2] Thus, the success of combinatorial chemistry in drug discovery is considerably dependent on further advances in heterocyclic MCR methodology, and according to current synthetic requirements, ecologically pure multicomponent procedures are particularly welcome. In this context, electroorganic synthesis has recognized as one of the methodologies that can fulfill several important criteria that are needed if society has to develop environmentally compatible processes.

Over the past 3 decades, the due to extensive research on electrochemistry of organic compound, electro synthesis become revolutionized technique for organic synthesis.[3] Electrochemistry has become an attractive alternative to conventional methods in organic synthesis, since only electricity is applied which might even originate from renewable resources, and therefore no reagent waste is produced.

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P-297

A convenient electro-catalyzed multicomponent synthesis of 4*H*-thiopyran derivatives

Rahul Dubey, Vinay K. Singh, Laxmi Kant Sharma, Abhishek Upadhyay, Narendra Kumar and Rana Krishna Pal Singh *

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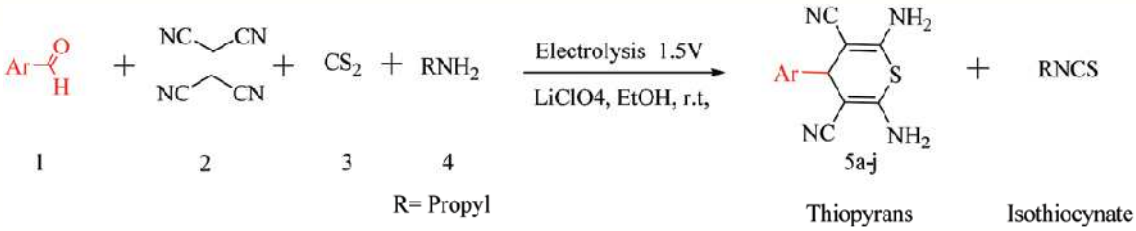
An environmentally benign synthesis of substituted 4*H*-thiopyrans was carried out by the condensation of aromatic aldehydes, malononitrile, carbon disulfide and primary amines. Constant potential electro synthesis was carried out in an undivided cell at room temperature in the presence of lithium perchlorate as a supporting electrolyte.



Electrochemical multicomponent reactions (EMCRs) have been used extensively to prepare bioactive heterocyclic compounds and became an important area of research in organic and medicinal chemistry.

The present work discusses the development of facile, simple, efficient, catalyst free methods for the synthesis of some 4H-thiopyran derivatives. The application of electricity as a reagent, use of simple solvents and supporting electrolytes are the special features of the reaction which makes it environmentally benign.

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P-298

Important Role of Hydrogen Bonding in Heteroleptic Iridium (III) Complex Interactions with Solvent, Dual Nature in pH Medium and Sensitive BSA Sensing

Vishal Kachwal, Amrit Sharma, Parva Sharma, Parvej Alam, Shibasish Chowdhury and Inamur Rahaman Laskar*

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Abstract:-

In this work we have used a Heteroleptic Iridium (III) complex containing 3-hydroxypicolinic acid as an ancillary ligand and phenyl pyridine as main ligand[1]. The complex is AIE active and emits near yellow region in solid state.Interestingly the emissive property of the complex depending upon both the polarity as well as the site specific interaction with different class of solvents. The complex show green emission in non-polar solvent, yellowish green in chlorinated solvent, bright yellow in polar aprotic solvent and the emission gets quenched in the polar protic solvent. Herein, we attempted to explain the structure property relationship of the complex to its surrounding environment. The presence of hydrogen bonding on the complex enables it to be multifunctional and probing the solvent dynamics, bases, pH and BSA (Bovine Serum Albumin) sensing (9.3 pM). All the mechanism has beenexplored with the help of various experiments and computational calculations (DFT, TD-DFT, Docking studies etc.,)[2,3].

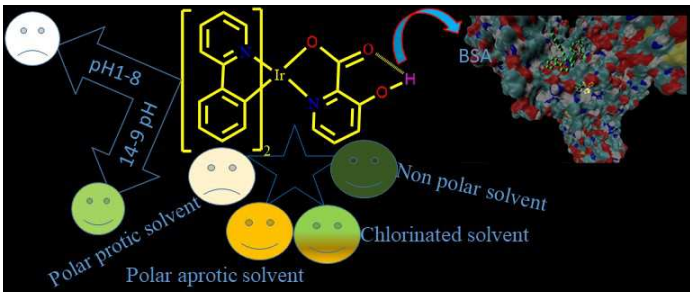

Figure 1 Schematic represntation of the complex interaction with surrounding medium (Solvent, pH and BSA (Bovine serum albumin))

Reference

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P-299

Synthesis and characterization of Cu (II) and Fe (II) metal complexes of Schiff base derived from O-Carboxymethyl Chitosan

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Abstract: The aim of present research work is to synthesize water soluble derivatives of chitosan. In this sequence, chitosan is treated with monochloroacetic acid to form O-Carboxymethyl Chitosan (O-CMC). Schiff base of O-Carboxymethyl Chitosan (O-CMC) have been synthesized by treating O-CMC with 4-fluorobenzaldehyde. Then metal complexes of Cu (II) and Fe (II) with Schiff base have been synthesized. These newly synthesized products were characterized by Fourier Transform Infrared spectroscopy (FTIR), ^{1}H-NMR spectroscopy and fluorescence study. The chitosan and its derivatives have applications in field of pharmaceuticals, agriculture and food preservation. All these products are water soluble and their antimicrobial activity have to be checked out.

Keywords: O-CMC, Schiff base, metal complexes

P-300

Identification of Lead Fragments for Designing Anticancer Compounds Based on the Energetics of Largazole Sub-Structures in HDAC8 Co-Crystals: Molecular Dynamics Approach

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Largazole, a secondary metabolite from marine flora *Symploca sp*., and its analogues are reported to show promising anticancer activity [1]. Largazole is closely related to Romidepsin (from *Chromobacterium violaceum*) an FDA approved anticancer drug [2]. The activity is attributed to their binding affinity to histone deacetylases (HDACs) responsible for transcriptional/ translational activity of the genetic material. Unlike in many small molecule inhibitors embedded with hydroxamic acid moiety, the side chain thiol group of largazole analogues acts as key functionality for binding with the enzyme using cofactor Zn^{2+} [2]. Traditionally natural products have served as a key source of scaffolds for new leads and for discovering therapeutic agents. Often the discovery of new leads involve constructionist approach, molecular fragment studies or metabolites analysis etc to determine the key constituents pertinent to the biological activity. The MD simulations of protein-ligand complexes provide a reliable estimate of dynamic characteristics and energetics of participating entities which can be used as indices to identify the lead fragments for designing new probable active compounds. In view of this, 20ns MD simulation were performed on co-crystal structure of HDAC8 with largazole analogues (PDB ligand id: L6G, L7G, L8G) to determine the dynamic characteristics protein-ligand complexes and energetics of intermolecular interactions [2, 3]. The average non-bonding energy between HDAC8 and ligands are broadly in agreement with reported inhibitory activities (L7G: -41.48 kcal/mol; L6G: -38.64 kcal/mol; L8G: -29.35 kcal/mol) [2]. The energetics of structural fragments of ligands computed from the simulations may serve in designing new or different inhibitors.

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P-301

Copper-Catalyzed Decarboxylative C-N coupling Reaction of α-Oxocarboxylic Acids with Isatins: A Facile Synthesis of 4H-Benzo[d][1,3]oxazin-4-ones

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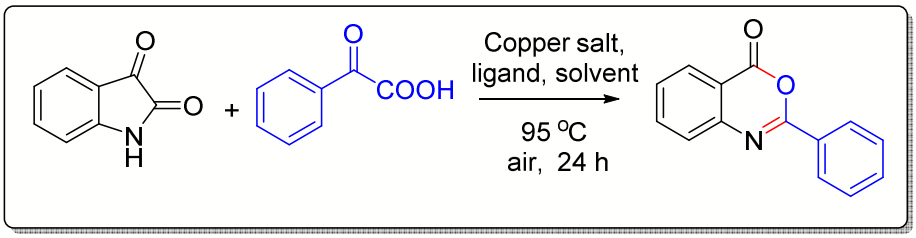
In past decade, the transition-metal-catalyzed decarboxylative coupling reaction has attracted a considerable interest in the C-C bond formation reactions [1]. 4*H*-Benzo[*d*][1,3]oxazin-4-ones are the key skeleton of many drug molecules and they show wide range of biological activities[2]. 2-Substituted 4*H*-benzo[*d*][1,3]oxazin-4-ones are the key starting material for the synthesis of pharmaceutically important compound.[3].Herein, we report an unprecedented copper catalyzed C-N coupling reaction of isatins with phenyl glyoxalic acids for the synthesis of benzooxazinones which proceeds *via* decarboxylation and decarbonylation reactions[4]. The broad substrate scope, high yield of products and functional groups tolerance reaction conditions are the noteworthy features of this reaction.



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P-302

Nano-titania modified agricultural waste for watertreatment

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Dyes removal from textile effluents on industrial scale has been given much attention in the last few years because of its potential toxicity and visibility problems. Numerous techniqueswere used in the recent past for removal of dyes [1]. Among them,photo-catalytic decompositionof dyes appeared as a promising method for decolouration of textile effluents [2].
Therefore, in the present investigations we extracted cellulose from wheat grass and modified its surface with nano-titania photo-catalyst. Degradation of an azo dye, methyl orange (MO), was tested in simulated wastewater with titania modified cellulose under visible and UV light. Samples were taken at various intervals and photo-catalytic activity was measured by UV–vis absorption spectroscopy. The observed results suggest that the titania modified cellulose act as an excellent photo-catalyst on the degradation of methyl orange as shown in figure 1.

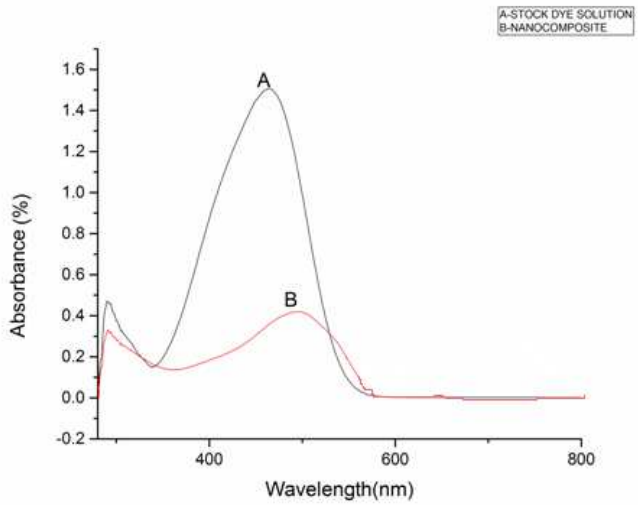

Fig. 1:UV-Vis Absorption spectra of methyl orangephoto-degraded by nano-composite.

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P-303

Encapsulation and Catalytic Study of "Ship-in-a-bottle" Palladium Schiff base Complexes Inside the Zeolite-Y

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ABSTRACT: A series of palladium Schiff-base complexes have been synthesized by using flexible ligand synthesis method[1] within the supercage of zeolite-Y. The encapsulation process usually converts these complexes into efficient catalysts with size and shape selectivity[2]. These complexes in both their free and encapsulated states have been characterised with the help of different characterization tools like X-ray diffraction patterns, SEM-EDS, XPS, IR and UV-Vis spectroscopy. The encapsulated palladium complexes have been employed as catalysts for Heck reaction and found more proficient compared to their neat states. All these encapsulated complexes have shown dramatic red shift of the charge transfer band in their electronic spectrum. On encapsulation within the supercage of zeolite Y, square planar Pd (II)–Schiff base complexes have shown modified structural parameters and high activity towards the Heck reaction. These heterogeneous catalysts can easily be separated from the reaction mixture and reused.

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P-304

Efficient and Sustainable Copper Catalyzed *O*-arylation of Nitroarenes with Substituted Phenols

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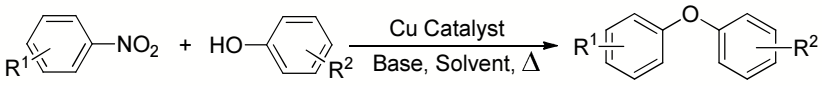
The arylethers are ubiquitous structural motif present in a variety of pharmaceuticals and functional materials. The transition-metal catalyzed C-O cross-coupling is a highly efficient and versatile method to access substituted arylethers.[1] In these reactions, aryl halides have originally been used as electrophiles in the presence of copper, palladium or iron-based catalyst. However, the use of aryl halides (a frequent environmental concern) causes undesirable halogen-based contamination, and the by-product generated during their coupling often hampers isolation and purification processes. Given the ubiquitous nature of arylethers in bioactive molecules and the drawbacks associated with their conventional synthetic methods, the exploration of alternative synthetic routes is highly desirable.

Activated nitroarenes are known to undergo nucleophilic aromatic substitution with metal-alkoxides or -aryloxides (strong nucleophiles) to give ethers under non-catalytic conditions.[2] However, these methods suffers from many drawbacks, including compatibility and harsh conditions. In contrast, the use of nitroarenes as pseudohalides in mild metal-catalyzed *O*-arylation may circumvent these problems and should be a useful alternative as nitroarenes are readily available and serve as building blocks for functionalized arenes.[3-4] Herein, we report a novel method involving the use of a copper-catalyst for the cross-coupling of nitroarenes with relatively non-nucleophilic phenols. The copper catalyst is easily isolable and can be reused for consecutive cycles without considerable decrease in yield and activity.



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P-305

Activation of C_{sp2}-Halogen Bonds Using Silica Immobilized Palladium Complex

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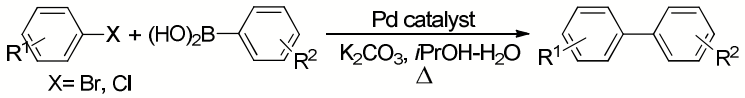
Transition-metal-catalyzed cross-coupling reactions are irrefutably part of the key reactions of organic synthesis, because they allow the construction of highly complex molecules from relatively simple precursors. The palladium-catalyzed Suzuki–Miyaura cross-coupling reaction of organic halides with organoboron compounds is one of the most powerful methodologies for the construction of C–C bonds, particularly for the synthesis of biaryls.[1-2] As part of our continuing efforts to develop functionalized silica-based palladium catalyst, we have developed a silica supported palladium complex and evaluated this new catalyst for the Suzuki-Miyaura cross-coupling reaction under aqueous media.[3-4] This solid complex is a highly efficient and easily recyclable catalyst for Suzuki-Miyaura cross-coupling reactions under mild aqueous condition, and can be reused efficiently up to 6th consecutive runs. The prepared catalyst was characterized by FT-IR, BET surface area measurements, XRD, SEM-EDX, EDS-mapping, ICP-AES, XPS and solid UV. The reaction proceeds under mild reaction conditions offering an environmentally benign alternative to the existing protocols.



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P-306

ANOMALOUS STRUCTURAL RELAXATION IN CHALCOGENIDE GLASSAND CRYSTAL: A CASE STUDY ON Ge20Te80MATERIAL

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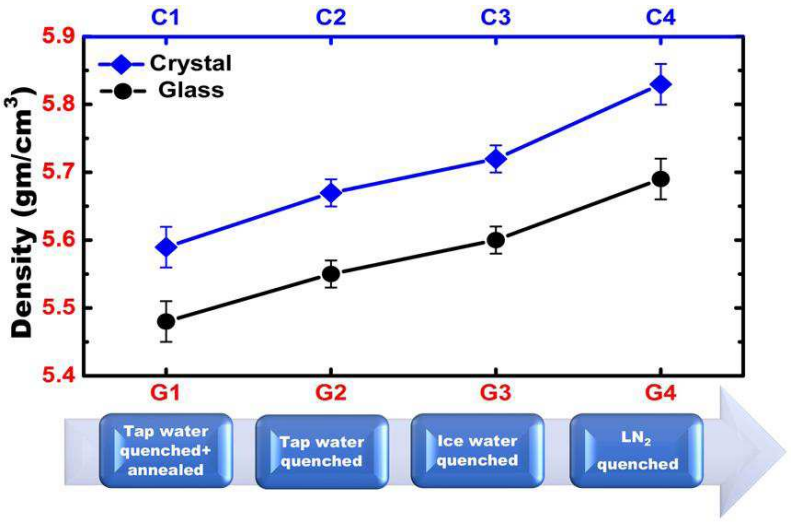
ABSTRACT: We found the deviations from an ideal behaviour of glass forming liquid of binary chalcogenide glass composition Ge20Te80 with respect to its quenching rate on mass density and thermal properties. Typically, the increase in quenching rate will decrease the characteristic relaxation time and correspondingly shift in the glass transition temperature (Tg) to higher temperature and result in lower density. This, however, holds only when the liquid structure remains same as in equilibrium glass structure independent of their quenching rate. We find Ge20Te80 glass composition with higher quenching rate is found to possess higher density and lower Tg than the lower rate quenched or well annealed glass specimen. In contrast to conventional glass forming liquids, the anomalous behaviour of Ge20Te80 glass with respect to quenching rate is closely related to the change in the local atomic structure with thermal history. Additionally, we found that crystal derived from the Ge20Te80 glass with different thermal history but with identical annealing conditions leads to different mass density, specific heat capacity, and local atomic structure. Thus, the observed unusual variations in the mass density and various thermal properties of Ge20Te80 glass and crystal are mainly linked with their corresponding local atomic structure and concentration of defect states associated with each state.



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P-307

Effect of temperature on corrosion combating efficiency of *Catharanthus roseus* extract on Al in HCl solution.

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Abstract

Extract of leaves of *Catharanthus roseus* was taken for studying its corrosion combating efficiency on Al in HCl solution. Weight Loss Method was employed for the studies. 1 M and 2 M HCl solutions were taken for weight loss studies. Inhibition concentrations were taken 0.1 % , 0.3 % , 0.5 % and 0.7 % in this method . Studies were carried out at 298 K and 308 K.

Results show that the corrosion combating efficiency of *Catharanthus roseus* decrease with rise in temperature . Maximum efficiency was found in 0.7 % concentration of inhibitor in 2 M HCl at 298 K and minimum was found in 0.1 % of inhibitor in 1 M HCl at 308 K.

Further result shows that corrosion combating efficiency of inhibitor increases with its increase in concentration.

Keywords: *Catharanthus roseus*, Weight Loss, Inhibition efficiency, Corrosion Rate, Surface Coverage.

P-308

Synthesis of fluorescent triazole by using β-cyclodextrin as a phase transfer catalyst

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Non-invasive techniques are increasingly gaining popularity amongst chemist, biologist and medical researchers for diagnostic purpose as they provide vital information with little inconvenience to patient. In line with this, fluorogenic click chemistry, which transforms a non-fluorescent compound into fluorescent entity is regarded as a powerful tool by the scientific community for the development of fluorophores. Recently, Triazole based fluorescent compounds are being explored owing to their acceptable fluorescence and excellent biocompatibility which makes them appealing fluorescent compounds in bio- imaging and in sensing various analytes. Keeping this view, we have synthesized a series of triazole *via* 1,3-dipolar cycloaddition reaction from coumarin azide and sugar alkyne in water in the presence of catalytic amount of β-cyclodextrin as a phase transfer catalyst. Highly fluorescent compound was obtained with absorption in ultraviolet region and emission in the green region. The compound will now be screened for wide range of biological activities and sensing of cations and anions.

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P-309

CuO NANOCATALYSED MULTICOMPONENT REACTION AS AN ADVANCE TOOL FOR SELECTIVE SYNTHESIS OF N-((3-METHYL-5-OXO-1-PHENYL-4, 5-DIHYDRO-1H-PYRAZOL-4-YL)(2-PHENYL-1H-INDOL-3-YL)METHYL)ACETAMIDE USING

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Abstract

Multi-component reactions in one pot using domino principle was assigned for the production of a new series of N-((3-methyl-5-oxo-1-phenyl-4, 5-dihydro-1H-pyrazol-4-yl)(2-phenyl-1H-indol-3-yl)methyl)acetamide derivatives by refluxing indole-3-carbaldehydes **(1a-f)**, 3-methyl-1-phenyl pyrazol-5-one **2**, in acetonitrile solvent **3** with drop wise addition of acetyl chloride **4** in the presence of various heterogenous base catalysts. CuO nanoparticles were distinguished as most effective and versatile catalyst among all tested catalysts. All the synthesized compounds were screened for IR, ^{1}H NMR, ^{13}C NMR, Mass spectra and elemental analyses.

P-310

Photo-Degradation of Some Textile Dyes using WO_3

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Abstract: The textile industry presents a global pollution problem owing to the dumping or accidental discharge of dye waste-water into waterways, which is having a major impact on the quality and aesthetics of water resources. The World Bank estimates that 17 to 20% of industrial water pollution comes from textile dyeing and treatment. During the last decade the Bhilwara has developed into a leading place in the textile industry in the country. Bhilwara is the hub of textile industries in the state of Rajasthan and known as "Textile City". Textile industry is one of the most water and chemical intensive industries worldwide. About 200-400 litres of water is needed to produce 1 kg of textile fabric in textile factories. Photo degradation of Textile dyes by WO_3 reagent has been investigated by using U.V. light in Photochemical Reactor at 254nm. The progress of reaction was observed spectrophotometrically. The effects of various parameters like concentration of catalyst, pH on the rate of degradation and decolourisation were also studied.

Key Words: Textile, WO_3 reagent, Bhilwara.

P-311

Synthesis and characterization of novel ionic compounds comprising of organic-inorganic framework

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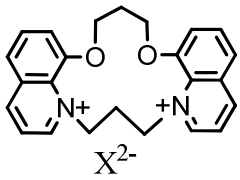
The design and synthesis of organic–inorganic hybrid materials had attracted considerable interest in the last few years not only from a structural point of view, but also due to their potential applications in different areas such as catalysis, medicine, sorption, electrical conductivity, magnetism and photochemistry[1-3]. In the present work novel ionic complexes comprising of cyclic organic cation [1,1-(Propane-1,3-diyl) -1, 3- Bis (1, 3 quinoxypropane) and inorganic anions as shown in fig.1 were synthesized and characterized by analytical methods viz. IR, NMR, Mass and elemental analysis. Structure of the compounds will be ascertained by single crystal X-ray.



$X = PF_6^-, Cr_2O7^{2-}, CoCl_4^{2-}, MnCl_4^{2-}$

Fig.1: The Proposed structure of the Complexes

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P-312

Synthesis of some new amine- thiourea based organocatalysts from substituted isothiocyanates

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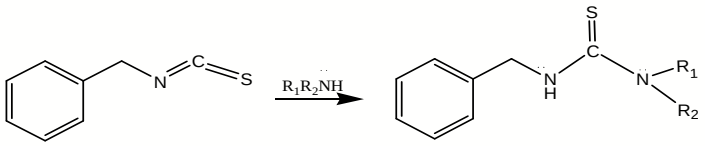
Over the past decade bifunctional compounds, bearing both a thiourea moiety and an amine group , have emerged as useful organocatalysts and found numerous applications for organic synthesis. Besides impressive developments with tertiary and secondary amine-thioureas[1,2]more recently, significant progress has been achieved with primary amine-thiourea organocatalysts. Demonstration of the potential of primary amine-thioureas as attractive new organocatalysts[3,4] has stimulated the interest of different research groups to develop new useful enantioselective transformations.The present study will give the details of the newly synthesized thiourea based organocatalysts with the help of different spectral studies.



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P-313

INFLUENCE OF VARIOUS CAPPING AGENTS ON OPTICAL AND ANTIMICROBIAL PROPERTIES OF SYNTHESIZED ZINC OXIDE NANOPARTICLES

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Abstract

The ZnO nanoparticles were synthesized by wet chemical route and change in morphology on changing the capping agent was studied.The synthesized nano-particles were well characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), UV-Visible spectroscopy, photo-luminescence and Dynamic Light Scattering (DLS) methods. Citric acid, Starch, PVP and Xylan capped ZnO particles showed better morphology and uniform size distribution than nanoparticles capped by PEG and chitosan. These synthesized products were then used to study the photo-catalytic effect in natural sunlight by degrading organic dye (methylene blue).It was observed that capping reduced the efficiency of photocatalysis in comparison to uncapped ZnO nanoparticle. The antimicrobial activity of ZnO nanoparticle against common gram positive and gram negative bacterial strains were also studied. Starch and PVP capped ZnO nanoparticles showed improved antibacterial activity over other capped nanoparticles.

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P-314

Synthesis and Characterization of selected coronene-porphyrins

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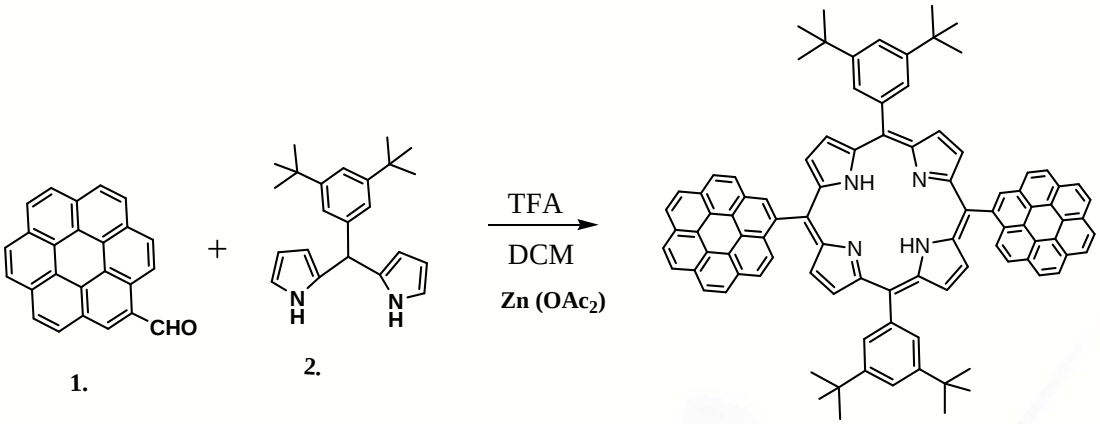
Abstract

Coronene is a π- planar polycyclic aromatic hydrocarbon with D_6h symmetry. Coronene was first synthesized in 1932 and isolated in 1955 from mineral Karpatite[1,2]. Coronene is smallest fragment of graphene in which all the C-C bond of the central benzene ring are shared with the peripheral rings. Hence the coronene is also called the super-benzene or nanographene[3]. The coronene has attracted much attention in material chemistry due to its relation to graphene. Polycyclic aromatic hydrocarbons substituted either at meso or peripheral position of porphyrins have been used in material and photodynamic therapy. Hence the synthesis of selected coronene porphyrins have been synthesized to understand their role in material chemistry and medicinal chemistry.

The reaction of coronene in carbon disulphide is treated with titanium tetrachloride and dichloromethyl Methyl ether followed by acidification with aqueous hydrochloric acid give the orange- yellow coloured coronene-aldehyde(1). Further reaction of coronene-aldehyde (1) with 5-(3`,5`- di-tertiary-butyl benze) dipyrromethane (2) in presence of acid gave the 5,15- di-coronenyl porphyrin(3). The structure of 5,15- di(coronenyl)- 10,20- di(3`,5`- ditert-butyl phenyl) is conformed by UV- Visible, ^{1}HNMR and other spectroscopic data. The reaction of above porphyrin (3) with Zinc acetate in CH_2Cl_2 to gave 10,15-bis-(3,5-di-tert-butylphenyl)- 5,15-bis(coronen-1-yl)-porphyrinato zinc(4). Thus an easy, low cost and in less steps synthesis of coronene- porphyrin has been achived.



1. 2.

3. X= 2H

4. X= Zn

P-315

Efficient Synthesis of Heteroarylporphyrins as Fluorescent Probes

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Porphyrins and metalloporphyrins are a distinct class of compounds utilized in various fields such as electron transport, catalysis, photodynamic therapy, optoelectronic devices and building blocks for supramolecular assembly[1]. Generally, porphyrin exhibits prominent absorptions in form of strong Soret band (380-500 nm) and weak Q bands(500-700 nm).For clinical applications in photodynamic therapy (PDT), it is desirable that the photosensitizer display absorption in the spectral region from 650 nm to 900 nm. Understanding the oxygen fluctuation in tumor cells is very important for the effective treatment of cancer. Porphyrin fluorophores have been explored in malignant cells for the visualization of fluctuation in oxygen concentration.π-Extension and π-expansion of porphyrins induces significant changein their photophysical properties [2].Particularly, π-extended porphyrinshave received greater attention in recent years due to their attractive properties including red-shifted absorption and emission profiles, intriguing non-linear optical properties and high electron mobilities[3].Porphyrins having extended π-system or conjugation with an appended peripheral heterocyclic moieties offer the possibilities for modulation of photophysical properties of the parent porphyrin. In continuation of our efforts to identify novel *meso*-substituted porphyrins [4], we have prepared various A_3B and A_2B_2 type's novel *meso*-substituted porphyrins by employing palladium-catalyzed cross-coupling reactions of haloporphyrins with azahetero cycles. Prepared hetero aromatic porphyrinsare characterized by NMR (^1H &^{13}C) and MALDI-TOF spectral data. Some of the hetero aromatic porphyrins displayed significant shift in absorption and emission bands. Couplingreaction conditions, reaction mechanism, characterization, and photophysical properties of the prepared porphyrins will be discussed during the conference.

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P-316

Bis(indolyl)keto-hydrazidehydrazones as Novel Tubulin Inhibitors

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Microtubules form crucial dynamic structural cellular components of the cell and are composed of the alpha and beta tubulin heterodimers. Microtubules are involved in a wide variety of functions in the cell such as attribution to cell shape, motility, intracellular trafficking, and mitotic spindle formation. Owing to these reasons, tubulin and microtubules have gained significant interest as important targets for cancer therapy. Tubulin targeting substances are broadly categorized into microtubule stabilizing (taxanes, epothilone, and discodermolide) and destabilizing (colchicine, Vinca alkaloids, cryptophycins, and CA-4P) agents [1] Indole skeleton is frequently found in many natural as well as synthetic chemical entities of immense biological significance. Among the indole-based heterocycles, bis(indole) alkaloids have drawn significant attention due to their diverse anticancer properties [2]. For example, Nortopsentins A-C, Topsentins, Hyrtinadine A, Coscinamides A-C were isolated from the marine sponges [3]. Bis(indole) containing linear chain spacers such as 1,2-diketo, glyoxylamide, enamide, hydrazide-hydrazones, have endowed with interesting biological activities in Coscinamides A-C, Hyrtiosin B. Indolic enamides like Igzamide, Didemnidine B, Indibulin showed good *in vitro* cytotoxicity against the panel of cancer cell lines [4]. Inspired by the potential of this naturally indoles, recently we have identified bis-indoles with 1, 2, 4-thiadiazoles, 1, 3, 4-oxadiazoles, α-cyano chalcones and hydrazide-hydrazone spacers as potent anticancer agents [5]. In continuation of our efforts to identify effective indole-based anticancer agents, herein we report novel bis (indolyl) ketohydrazide-hydrazones by incorporating a ketohydrazide-hydrazone scaffold between the two indole rings while maintaining the crucial features of coscinamide, indibulin and bis (indolyl) hydrazide-hydrazones. Various ketohydrazide-hydrazones were prepared from the reaction of indolyl glyoxalylhydrazide with appropriate aldehydes. Some of the ketohydrazide-hydrazones were found to exhibit significant *in vitro* anticancer activity with IC_{50} values in nanomolar range against a panel of cancer cell lines. Details about synthesis and anticancer activity study of ketohydrazide-hydrazones will be discussed during the presentation.

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Detection of Hg^{2+} ions in Aqueous Medium Using an Indole-Based Fluorescent Probe: Experimental and Theoretical Investigations

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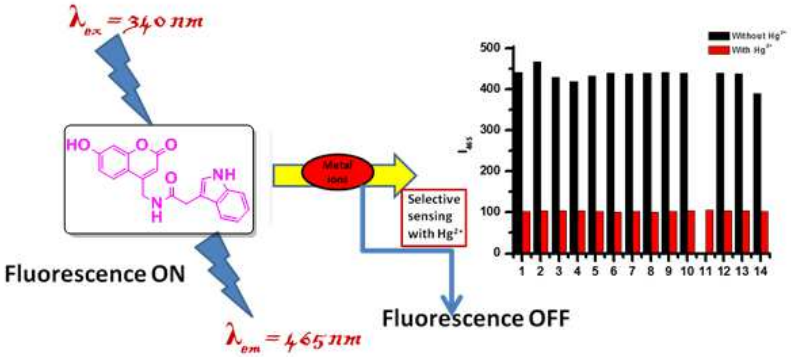
Abstract: Mercury pollution is a widespread danger to human health and environment.[1]Due to limitations associated with the existing Hg^{2+}chemosensors, development of new, efficient, selective chemosensors capable of sensing mercury ions in aqueous medium remains a demanding area of research.In this regard, an indole-based fluorescent probe has been synthesized and characterized by detailed spectroscopic analysis. The probe showed a high selectivity and sensitivity towards Hg^{2+} by giving significant fluorescence quenching over other tested cations in H_2O/DMF (7:3, v/v) medium. The association constant (K_a) wasfound to be 6.4×10^3 M^{-1} between sensor and Hg^{2+}. Detection limit was found to be as low as 0.143 µM (143 nM), which is far lower than the maximum level for mercury of 0.01 M in drinking water from Environmental Protection Agency (EPA) guidelines.Various spectroscopic analysis of probe and its Hg^{2+}-complex were performed to identify the possible binding interaction of the Hg^{2+} ion with the probe, which were further verifiedwith Density Functional Theory studies.[2]



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P-318

Organocatalytic asymmetric synthesis of Indolyl-piperidines and related alkaloids

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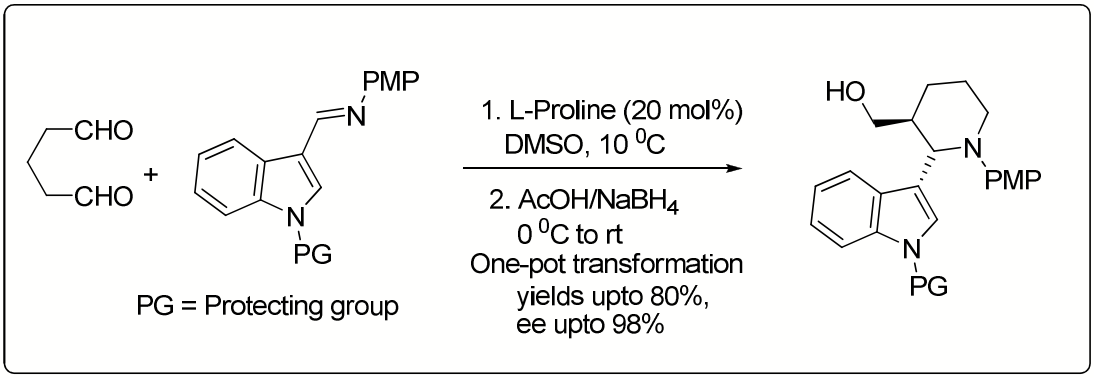
Indoles are widely distributed in several natural products and drug molecules as a common core skeleton [1]. Indole derivatives, in particular enantioselective functionalized indoles are attractive scaffolds for design and synthesis of various biologically important molecules [2]. Though the synthesis of chiral indole-3-pyrrolidines is important [3], the synthesis of chiral indole-3-piperidines is also equally important and considered as a challenging task, because of these attractive synthetic molecules accesses several natural products and valuable synthetic compounds [4]. Here we present our contribution towards the synthesis of chiral indole-3-piperidines through organocatalytic [4+2] annulation/reductive cyclization of glutaraldehyde with various indole-3-imines in detail here. (Scheme 1)



Scheme 1: Organocatalytic [4+2] annulation/reductive cyclization for the synthesis of chiral indole-3-piperidines

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P-319

Organocatalytic enantio selective synthesis off used 1,2-dihydropyridines *via* formal[4+2]cycloaddition between aqueousglutaraldehyde and dibenzo[b,f][1,4]oxazepineimines

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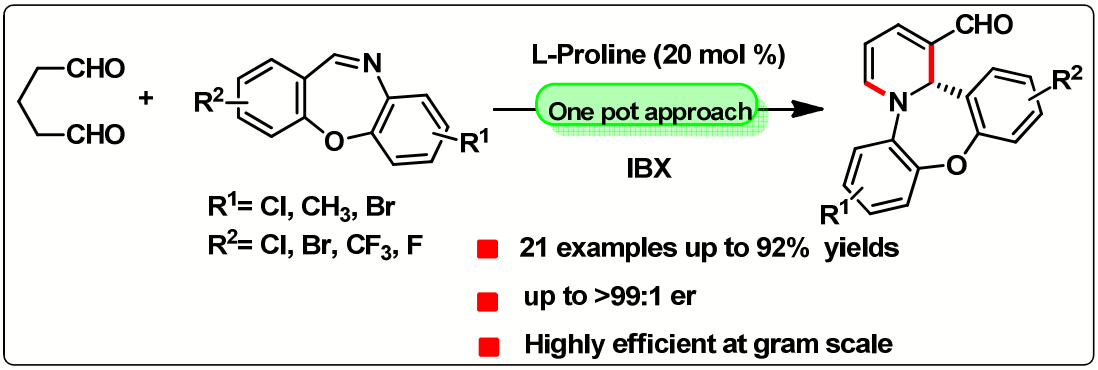
Abstract: Dihydropyridines (DHPs) are frequently encountered in natural and synthetic compounds that possess many interesting biological activities.[1]On the other hand, The dibenzo[b,f][1,4]-oxazepine scaffolds are core structures in numerous biologically active compounds.[2]Some of these derivatives also exhibit anti-HIV, anti-tumor and anti- inflammatory activities.[3]Thus, the 1,2-Dihydropyridine-fused dibenzo[b,f][1,4]oxazepines might exhibit impressive bioactivities. In continuation of our interest in organocatalyzed reactions,[4] we recently developed an efficient organocatalytic asymmetric method for the synthesis of 1,2- Dihydropyridines (DHPs) using aqueous glutaraldehyde and imines with high yields and excellent enantioselectivity[5]. Here, we present a new method for the asymmetric synthesis of fused 1,2-dihydropyridines via formal [4+2] cycloaddition between aqueous glutaraldehyde and dibenzo[b,f][1,4]oxazepine imines**(Scheme 1).**



Scheme 1: Organocatalytic asymmetric synthesis of dibenzo[b,f][1,4]oxazepinefused 1,2-DHPs

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Investigation of Thermal charging ability of Nanocomposite embeded PCM for Solar Thermal energy application

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A stable salt hydrate based PCM composite has been prepared using silver and grapheme oxide and used for the investigation of thermal charging ability. Grapheneoxide was prepared using the modified Hummers method. The composite was prepared using melt mixing scheme, which consist two steps. Nanomaterials were dispersed into the molten PCM with variable concentrations, followed by a strong shear mixing with a magnetic stirrer for 15 min, and ultrasonicatied for 45 min. The NPCM suspensions were poured into a mold, and then allowed to solidify at ambient temperature ($25^{O}C$) to form solid composites. In this way, nanomaterials-based NPCM composite was prepared. Prepared composite was characterized using SEM. The melting of PCM and NPCM composite was carried out on a convention heating system. From melting and solidification curves it is observed that the starting of the melting of PCM composite starts ~ 28 minutes. The NPCM demonstrated the fast and uniform heating as compared to pristine PCM. Lower time (22 min) for composite PCM to reach their melting point is mainly due to enhancement in the thermal conductivity of PCM due to the presence of high thermal conductive graphene oxide and silver nanoparticles. Varying proportion of the nano composite was used for this analysis and the thermal conductivity is maximum at 0.6 mass % of composite.

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An Efficient One-Pot Synthesis of Oxadiazolylporphyrins

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Porphyrin and its derivatives have received a considerable attention with their applications in diverse fields such as optoelectronics, photosynthetic systemsand catalysis[1]. *meso*-Appended porphyrins were used in the construction of multi-linked porphyrin assemblies that have shown various utilities in the development of molecular switches[2].Photophysicaland electrochemical properties can be tuned by the modification on either *meso*or*β*-peripheral position of porphyrin macrocycles,which displayed diverse and intriguing properties depending on the fusion patterns and/or the intrinsic nature of the embedded heteroatoms[3].In some of the reported porphyrinoids, structural modifications at *meso*-position led to absorption near IR region (~ 420-450 nm) with enhanced fluorescence profiles (650-750 nm) and redox potentials[4]. These applications in electro-optics require efficient overlapping of *π*-electrons which could beachieved by linking one or two electron donating moieties in the *meso*-positions [5].In continuation of our efforts, we have developed the synthesisof oxadiazolylporphyrins by the oxidative cyclization of*in situ*generated porphyrinhydrazonesinvolving the reaction of formylporphyrinwith variousarylhydrazides.Prepared heteroaromaticporphyrins were characterized by theirUV, NMR and MALDI-TOF spectral data and found to display interesting absorption and emission properties. Synthetic details along with photophysical properties of the *meso*-appended oxadiazolylporphyrinswill be discussed during the conference.

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Diaryliodonium Salts-PromotedArylation of Quinolones

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Quinolone derivatives are important and general building blocks which are suitable precursors for many biological compounds,including pharmaceuticals, medicine, andagrochemicals [1]. Owing to interesting biological profile, many groups have been reported the functionalization at various positions of quinolonescaffold. In thiscontext, very recently we have demonstrated*N*-/*O*-arylation of quinolone under metal-free conditions [2]. Similarly, C-2 and C-3 arylation of quinolone have been disclosed by other groups using haloarenes or arylboronic acids in presence of variousmetal-catalysts such as Ru, Rh, and Pd [3]. However, C-5 arylation of quinolonehas not been explored till now. On the other hand, C−H functionalization has received considerableattention due to rapid derivatization of drug-like molecules.The catalytic site-selective arylation of unreactive C–Hbonds is an area of great importance for the designof atom economical approaches to prepare useful organicmolecules. In this ambient, the “directing group” strategy has been one of thepopular methodologies to address issues of selectivitywhereby pre-existing functionality within a molecule candirect a metal catalyst to unreactive position for insertion [4]. In recent years, diaryliodonium salts occupied a very important role as arylating agents in many coupling reactions due to their relatively benign character,stability, high electrophilicity, less toxicity, and recyclability [5]. Due to potent pharmacological features associated with arylated heterocycles, we have developed the synthesis of 2-arylindoles, diarylsulfones, and arylated azaheterocyclesusing diaryliodonium salts [6]. In the light of significant properties of quinolones and utilities of diaryliodonium salts, herein we have developed a site-selective palladium-catalyzed C-5 arylation of quinolones by utilizing diaryliodonium salts. Prepared arylquinolones are characterized by NMR (^{1}H &^{13}C), IR and mass spectral data. Details about the reaction optimization, synthetic strategy, and mechanistic pathway will be presented in the conference.

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Molecular Iodine Mediated EfficientSynthesis of PityriacitrinAnalogues*via* Intramolecular Cyclizationof Bis(indolyl)ketoamides

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Development of simple and efficient synthetic approaches to access diverse marine natural products are highly valuable for their wide presence and indispensable role in pharmacologically active agents and the valuable therapeutic entities[1].For example, β-carboline alkaloids are one of the significant class of marine-derived secondary metabolites, with wide occurrence amongst a variety of marine sources such as sponges, tunicates, algae, worms, and microorganisms. β-Carboline alkaloids have been extensively studied for their broad range of bioactivities including antimicrobial, antiviral, anti-HIV, p56 tyrosine kinase inhibition, antimalarial, anti-angiogenic, antiproliferative activity against numerous cancer cell lines and action as a DNA intercalators[2].Despite the high importance of β-carboline alkaloids in medicinal chemistry, limited synthetic methods for the preparation of β-carboline natural products especially, pityriacitrin analogues are reported[3].Moreover, there are still limitations associated with reported protocols such as multistep synthesis, limited substrate scope, and low yield. Therefore, more general and eco-friendly procedures for the synthesis of pityriacitrins from easily available starting materials are still highly desirable. Our interest in indoles and their analogues for extended biological assays[4]has promoted us to explore a simple and more efficient methodologyfor the preparation of pityriacitrin analogues using indoles as starting materials by employing triphenylphosphine and molecular iodine-induced dehydrative cyclization under mild reaction conditions. The developed approach is general and operationally simple and expands the synthetic utility of bis-indolyl ketoamides for the synthesis of a variety of 1-indoloyl *β*-carbolines which are of great importance in medicinal chemistry as well as in natural products. Furthermore, this reliable method applied for the preparation of naturally occurring *β*-carbolines like Pityriacitrin, Pityriacitrin B, hyrtiosulawesine, and Alangiobussinine. Detailed reaction conditions, characterization and a prepared library of 1-indoloyl-β-carbolines will be presented during the conference.

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P-324

Design and synthesis of novel biodegradable polymers

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INTRODUCTION: During the past few decades, and more importantly in the last decade, significant advances have been made in the development of biodegradable polymeric materials for various applications.The idea of biodegradable plastics is of significant enthusiasm concerning strong waste amassing. More prominent endeavors have been made in creating degradable natural materials with no ecological contamination to supplant oil-based conventional plastics. Among various sorts of degradable polymers, polylactic acid , commonly known as called polylactide, (obtained from corn starch) an aliphatic polyester and biocompatible thermoplastic, is right now one of the most encouraging and prevalent material with the brightest improvement prospect and is considered as the 'green' eco well -disposed material. Biodegradable plastics like polyglycolic, polylactic, polycaprolactone, polyhydroxybutyrate etc. are economically accessible for controlled medication discharges and also other applications.

In view of the wide range of applications of biodegradable or green polymers, the objective of the present research paper is to explore other economically viable and ecofriendly raw materials for the design and development of novel biodegradable polymeric materials and also modify the existing biomaterials to encorporate the desired properties in them.

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Synthesis of 4'-methyl-6'-substituted aristeromycins

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Abstract

4'-methyl-6'-substituted aristeromycins were synthesized from D-ribose**.** The key features of its preparations are: i) Ring opening with Grignard reagent produced highly stereo selective acylic carbon skeleton of diol; ii) 1,6-enyne reductive cyclization using $Rh(COD)_2BF_4$ and BINAP in presence of H_2at ambient temperatureafford stereospecific keycarbocyclic sugars ; and iii) the coupling with purine derivative by a Mitsunobu reaction.

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P-326

Computational unravelling of the role of alkyl groups on the host-guest complexation of pillar[5]arenes with neutral dihalobutanes

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Abstract: DFT calculations have been carried out to understand the electronic structure and non-covalent interactions within host-guest complexes between 1,4-dihalobutanes (DHBs) and alkylated pillar[5]arenes. Binding energies show that the propyl substituted pillar[5]arenes are found to have greater binding abilities than that of pillar[5]arene with smaller alkyl chains. Among the halogens, dibromobutane is found to have higher binding energy compared to difluoro and dichloro butanes respectively. Contribution of different molecular units towards the frontier molecular orbitals has been studied to gain insights into the role of each segment at the molecular level. Electrostatic potential maps of bare host pillar[5]arenes and their inclusion complexes with DHBs are investigated to draw clues on the nature of active sites for the inclusion phenomena. Non-covalent interactions present in these host-guest complexes are addressed from NCI analysis based reduced density gradient method. In order to characterize these weak interactions, Bader's Quantum Theory of Atoms In Molecules (QTAIM) analysis is utilized to differentiate the nature of non-covalent interactions present in these inclusion complexes. Our results reveal that though the hydrogen bonding patterns in pillar[5]arenes inclusion complexes are collapsed upon alkylation, a new set of X---H-C interactions stabilize these DHBs along with other C-H---π interactions in the alkylated pillar[5]arene inclusion complexes. Overall, the present study sheds light on the importance of the alkyl chain and handling non-covalent interactions carefully to tune the binding ability of pillar[5]arenes.

Keywords: Pillar[5]arenes, inclusion complexes, DFT, QTAIM and NCI-RDG.

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P-327

Synthesis of 4-amino-phenol derivatives of isoquinoline via iodine mediated imination/benzylation/aromatization of 1,4-cyclohexanedione

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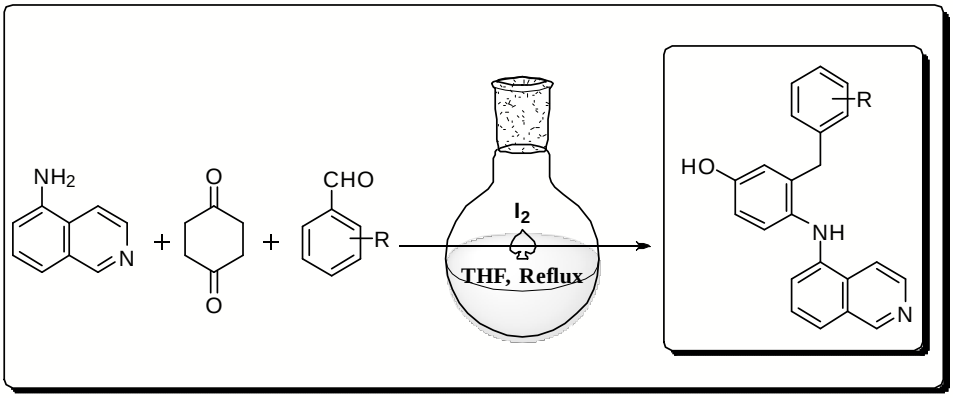
Abstract: Multicomponent reactions (MCRs) are vital tool for the synthesis of biologically important complex scaffolds. In addition, MCRs have gained remarkable importance due to their high productivity and operational simplicity for the construction of biologically active heteroaromatic molecules.[1] In continuation to our labs interest towards identification of new antiparasitic scaffolds, herein, we have developed a multi-component domino metal free approach for the synthesis of 4-hydroxy-2-benzyl substituted amine derivatives of isoquinoline. The three component domino reaction of 1,4-cyclohexanedione (phenol precursor), heterocyclic amine and benzaldehyde (benzyl precursor) catalyzed by molecular iodine afforded benzylated 4-aminophenol derivatives of isoquinoline moderate to good yield.



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P-328

Socio-economic Causes of Fluorosis in Rural Areas of Jahazpur, Bhilwara (Rajasthan) India

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ABSTRACT: Excess intake of fluoride causes dental and skeletal fluorosis and other ill effects on human health and slowly it makes a working, productive and healthy human being to a disable, unproductive and burden on society. Problems of fluorosis are becoming for population across the globe including India. In India many states including Rajasthan seriously affected with water born diseases in which fluorosis is major. The major sources of fluoride in water are geogenic and anthropogenic but intake of fluoride through drinking water not only depend on water quality, geography of area but socioeconomic status, literacy level, nutrition level, availability of facilities to population also. In rural parts of Jahazpur, Bhilwara (Rajasthan) the fluorosis is mainly linked with socioeconomic status; People of poor and socially weaker section of society are more affected comparatively than others. This paper mainly focused on the sources of fluoride in drinking water and the factors favouring in increase of fluorosis in rural parts of Jahazpur, Bhilwara (Rajasthan) Rajasthan.

Keywords: Fluoride, Dental fluorosis, skeletal fluorosis, Geogenic and Anthropogenic

Figure 1:- Dental and Skeletal Fluorosis in rural parts of Jahazpur, Bhilwara (Rajasthan) India

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P-329

Spectrophotometric Studies of the Charge Transfer Complexes formed between Pyridine and its Amino Derivatives (Donor) and DMAD (Acceptor)

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ABSTRACT

Nitrogen-containing heterocyclic compounds are of special interest as they behave as n- as well as π electron donors. Charge-transfer complexes of Pyridine and its amino derivatives are widely used by the pharmaceutical, textile, agricultural and other industries. A number of reports have been found pertaining to the formation of charge transfer complexes of amino and halogen substituted pyridine with suitable acceptors i.e. chloranil, malic-anhydride, α-nitroso-β-naphthol etc. A very few reports have been found involving the formation of charge transfer complexes of picolines (methyl pyridines) as a donor. Keeping in view, in the present work, formation of charge transfer complexes between the pyridine/picoline and theirs amino derivatives (donor) and dimethyl acetylenedicarboxylate (DMAD acceptor) have been investigated. The stoichiometry of the synthesized CT complexes was determined by mole ratio method spectrophotometrically and found to be 1:1. The appearance of the new wavelength band above 500 nm associated with colour change from colourless to red was observed. The formation constant and molar extinction coefficient of each synthesized charge transfer complex was also determined using Benesi-Hildebrand equation. The high value of formation constant of 2-amino-4-picoline was confirmed the high stability of the complex formed between it and DMAD and attributed to the high donation power due to the presence of two electron donating groups i.e. methyl and amino groups.

Keywords: Charge transfer Complexes, Pyridine, Picoline, Mole-ratio method, Benesi-Hildebrand equation

P-330

Multicomponent Domino reaction towards Synthesis of Pyrazolo/Isoxazolodihydropyridine and their Evaluation as Antileishmanial agents

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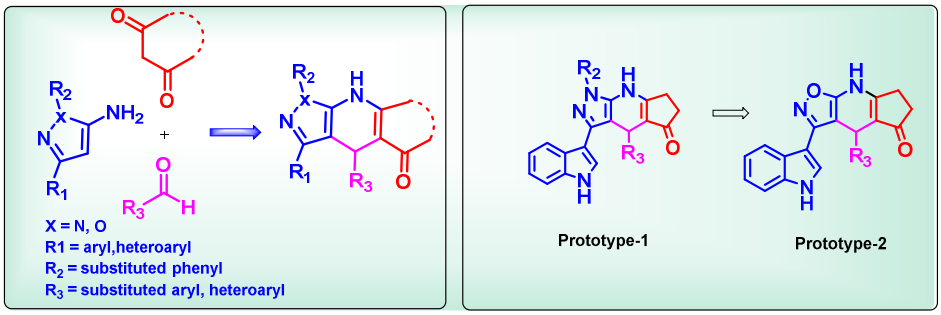
Multicomponent domino reactions (MDRs) can offer easy access to useful multiple functionalized ring structures of chemical and pharmaceutical interest.[1]Dihydropyridines and their congeners have gained considerable attention due to their wide range of biological activities such as antibacterial, calcium channel blocker, anti-proliferative, antitumor and antileishmanial agents.[2,3]Based on literature reports on nitrogen heterocycle as privileged anti parasitic agents pyrazolopyridinehave been designed and synthesized by MCR.[2] One of the compounds has displayed*in-vivo* activity at a dose of 50mg/kg. Further structural simplificationled to Prototype-2 with *in-vitro* potency against visceral leishmaniasis.



Keywords: Multicomponent Domino Reaction, Dihydropyridine, Isoxazolodihydropyridine

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P-331

ALTERNATIVE MEDICINE

Tarun Maheshbhai Patel, Ripal B Patel, Jaimin B Patel

Herbal medicine shows that healing is approached from a holistic framework. They remains one of the major strength of tribal religion. Herbal medicine is now being recognize in mainstream. Herbal remedies date back to a burial site some 60000 year ago when Nenderthal man was found with plant pollen and eight other plans placed around the dad man. Seven of the eight plants are still used in the herbal world today. All cultures are aware of the benefits of herbs but one district culture to lend amount of herbal pharmacopoeia to the 20 century are the native ameicans. Currently, about one fourth of all sold in American .Today contain at least on ingredient from plant material.

P-332

Generation of Electrical Energy from Solar Energy by Dye Sensitized Solar Cell

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ABSTRACT

Solar energy is the energy obtained by capturing heat and light from the Sun. Energy from the Sun is referred to as solar energy. Technology has provided a number of ways to utilize this abundant resource. It is considered a green technology because it does not emit greenhouse gases. Solar energy is abundantly available and has been utilized since long both as electricity and as a source of heat. The solar energy is the energy obtained by capturing heat and light from the Sun. The method of obtaining electricity from sunlight is referred to as the dye sensitized solar cell. Dye sensitized solar cell is device in which solar energy convert into electrical energy via formation of energy rich species that exhibit the PG-effect. PG-effect was studied in dye sensitized solar cell is consisting of photosensitizer (Fuchsin Basic) dye with aqueous solution of reductant (Mannitol). The observed cell performance in terms of maximum value of photoelectric parameters, conversion efficiency and storage capacity. The electrochemical properties of fuchsin basic dye at concentrations lowest and highest of Mannitol are distinctly different. The conversion efficiency and performance of the cell is observed 0.744% and 90 minutes respectively. Present work is the effort to generation of electrical energy from solar energy by dye sensitized solar cell.

Keywords: - DSS cell, PG-effect, conversion efficiency and storage capacity.

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P-333

Microbial Assisted Transformation A Novel approach

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Abstract

Microbial transformation provides novel highly selective and greener processes, as well as novel potential chiral synthons for the pharmaceutical and fine chemical industry.In organic synthesis the use of enzymes and microorganisms can avoid not only unwanted side reactions but also provide less hazardous and less toxic products as compared with conventional chemical catalysts. Microbial transformation is a convenient and useful synthetic route due to its high efficiency, mild and environmental friendly operation conditions, high selectivity, low energy consumption, ecofriendly nature, low cost, easier handling, yield minimum byproducts, can be reused and synthesis of chiral compounds. Many of these synthesized compounds have potential antibacterial properties against the pathogenic bacteria.

Keywords: Microbial transformation, Eco-friendly, Antibacterial properties, Chiral compounds

P-334

Artificial Neural Network Modeling (ANN) for the Biosorptive removal of Cu (II) and Cr (VI) ions using acid modified *Tamarindus indica* biomass.

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Abstract:

An artificial neural network (ANN) model was developed to predict the removal efficiency of copper (II) and chromium (VI) ions from aqueous solution using acid treated *tamarindus indica* biomass as an adsorbent. The three layer architecture model of ANN with simple back propagation algorithm was premeditated for the study. The biosorption data of Cu(II) and Cr(VI) ions, collected from laboratory experiments were supplied as an input /independent parameters to the prearranged ANN model. The input parameters of the models were shaking speed, initial concentration, adsorbent dose, temperature, time, and pH. The output parameter was biosorption capacity, qe. In the present study, four different acids viz. oxalic acid, succinic acid, maleic acid and tartaric acid were chosen for modifying the biomass The model worked with two transfer functions: tangent sigmoid (input layer to hidden layer) and linear transfer function (hidden layer to output layer). The model had 10 neurons in hidden layers which were registered on the basis of minimum RMSE (root mean square error). Among four acids, succinic acid gave the excellent results with high qe value. The high correlation coefficient between the theoretical and the experimental data has proved ANN model as a significant mathematical and computing model to predict the removal of efficiency of copper (II) and chromium (VI) ions from aqueous solution using *tamarindus indica* efficiently.

Keywords: Biosorption; *tamarindus indica*; chromium (VI), copper (II), tangent sigmoid, linear transfer function

P-335

Construction of Tale Nucleases for Site-Specific Cleavage of TheHuman Genes

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Abstract

Co-regulated genes require chromosomal contact to form a long distance multigene-complexes. Such wide range chromosomal interactions are lost in gene ablation studies investigating role of either transcription factors or interaction of chromatin structures. Whether such chromosomal contacts are absolute necessity for the transcription, we used Transcription activator-like effector nucleases (TALENs) restriction enzymes that can cut specific sequences of DNA thereby disrupts the contacts within multigene complexes. Such disruptions induced by TALENs was visualized using RNA FISH and highlighted the direct contact dependent co transcription of member genes of a complex. This report suggest that chromosomal contact have much more greater effect on co regulated genes within a complex.

P-336

Computational tuning of electronic and geometrical effects on Cobalt $PY5Me_2$ based molecular electrocatalyst

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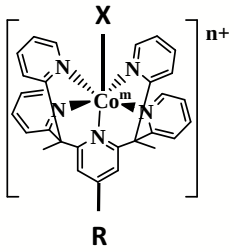
Abstract

The design of more efficient molecular electrocatalyst is pivotal for the development of renewable energy sources such as hydrogen molecule. In this connection, cobalt based molecular electrocatalyst with diverse ligand skeletons (Especially N_4PY5Me_2, N_5PY5Me_2) are found to acquire, robust and active catalyst for H_2 generation. The stability and catalytic activity of the molecular cobalt pentapyridine could be easily tuned upon changing the suitable substituents on the ancillary $PY5Me_2$ scaffold. This kind of work would help us to understand the molecular origin of catalysts. Further, changing the substituents on the $PY5Me_2$ scaffold will not only alter the over potential for hydrogen evolution and also affect the stability of the catalyst. So, it is important to understand the electronic effect of different substituents of $PY5Me_2$ ligand skeleton. In this connection, we are aiming to perform detailed quantum chemical calculations on cobalt pentapyridine catalyst for proton reduction with different substituents (Chart-1). Mainly, focus to obtain the proper correlation between structural and reactivity of these complexes via computed spectroscopic (UV and EPR) bonding and electrochemical data with experimental findings. In this poster, we are presenting the findings related to above aspects.



R=(H, CH_3, OCH_3, NCH_3, CF_3, F, Cl, Br, CN, NO_2, NH_2)
X=(CH_3CN, CH_3COO^-, H)

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P-337

Role of Chalcones as Michael Acceptor : Synthesis of Some Benzimidazolyl Pyrazoline Carboxaldehydes Under Microwave Irradiation and Their Antimicrobial Screening

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ABSTRACT

Michael condensation has been carried out for the synthesis of some 3-benzimidazolyl- 5-aryl-2 –pyrazoline –1-carboxaldehyde is based on microwave assisted solid phase, solvent free protocol. In the present study, condensation between benzimidazolyl chalcone and hydrazine hydrate has been carried out in presence of formic acid and basic alumina.The required benzimidazolyl chalcones were obtained by Claisen-Schmidt condensation under MWI irradiation. The synthesized compounds were tested for their antibacterial and antifungal activity in vitro.

Keywords: Michael condensation, solvent free protocol, Claisen-Schmidt condensation.

P-338

Synthesis and antitumor evaluation of novel pyrrolo [2,1–*a*]phthalazine derivatives

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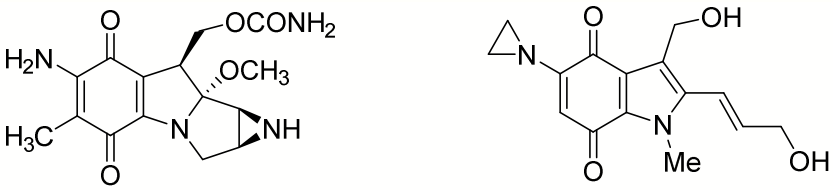
Cancer is the major leading causes of death in the world. Therefore, the design of new antitumor agents is one of the most challenging task in research areas of medicinal chemistry. For the treatment of various cancer patients, naturally occurring Mitomycin C (MMC, 1) is a clinically useful chemotherapeutic agent amongst DNA alkylating agents.[1](Figure 1)

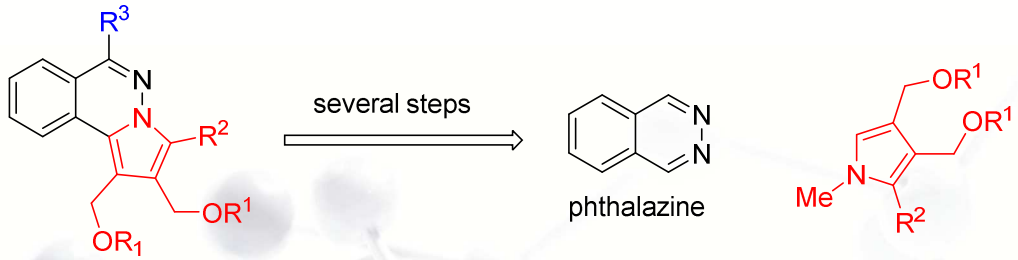


1 Mitomycin C (MMC) **2 E09**

Figure 1 Mitomycin C and its analogue

Indoloquinone EO9 (2)[2], a synthetic analogue of MMC which possess two reactive nucleophilic centres was reported to be capable of DNA cross-linking. The quinine part of these agents plays significant role in their antitumor activity, which requires bioreductive activation to switch on the nucleophilic centres on the pyrrole ring to allow interaction with DNA.[3]

In view of these potential nature of the compounds, it was thought worthwhile to study the effects of hybrid molecule consisting of two pharmacophoric moieties like phthalazineand bis(hydroxymethyl)pyrrole in a single molecule. Herein we report synthesis, characterization and biological evaluation of novel pyrrolo[2,1–*a*]phthalazine derivatives. Detailed characterization including ^{1}H NMR, ^{13}C NMR, HRMS and *in-vitro* study for all newly synthesized compounds and *in-vivo*study of active molecules has been reported.



>30 compounds
upto 90% overall yield
***in-vitro* and *in vivo* studies**

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P-339

ONE-POT SEQUENTIAL APPROACH FOR THE CONSTRUCTION OF HIGHLY FUNCTIONALIZED TRIAZOLO[4,3-c]PYRIMIDINES.

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Abstract:

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 acylketene dithioacetals and arylamidines. Moreover, this process describes the application of presynthesized arylamidines, which omits the Suzuki-Miyaura cross-coupling reaction and hence provides metal-free organic synthesis in an atom and step economical fashion.

P-340

Synthesis and Characterization of highly Substituted Pyrazolo[1,5-a]Pyrimidines.

Ashokbhai Rathod, Dhananjay Pandya, Mayur Shiyal, Prof. Y. T. Naliapara*

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Abstract:

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)-1H-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.

P-341

One-Pot Synthesis of Fully Substituted Pyrimidines Using Amidine and Ketene dithioacetals as Synthons.

Mayur Shiyal, Dhananjay Pandya, Ashok Rathod, Prof. Y. T. Naliapara*

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Abstract:

A simple, convenient and efficient one pot synthesis of fully substituted pyrimidines was developed by cyclocondensation of α-oxo ketene dithioacetals with amidine in the presence of potassium carbonate in good yield. Structures of all the newly synthesized compounds were elucidated by elemental analysis and spectral analysis.

P-342

Use of cyclic aliphatic ketones for spiro 2-amino-3-cyano pyrano[3,2-c]chromene formation

Bhola Yogesh, Prof. Y.T.Naliapara

Abstract

The three component reaction between 4- hydroxycoumarin, malononitrile and carbonyl compounds in ethanol in the presence of morpholine as a catalyst was studied. Only cyclic aliphatic ketones afford spiro 2-amino-3-cyanopyrano[3,2-c]chromene derivatives.

P-343

Potassium *tert*-Butoxide Catalyzed Three Component Domino Reaction Strategy: Synthesis of Triazolo[5,1-b]quinazoline and Benzimidazo [2,1-b]quinazoline Derivatives.

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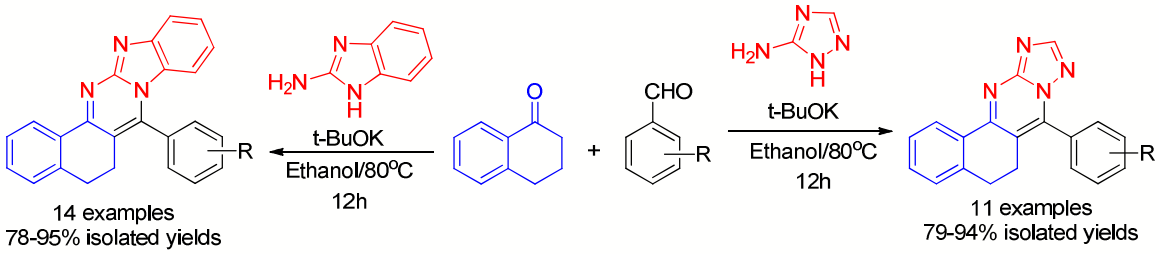
Abstract: Three-component reactions of α–tetralone with 1,2,4-triazol-5-amine/2-aminobenzimidazole and aromatic aldehydes have been discovered by using potassium *tert*-butoxide (*t*-BuOK) as a catalyst. A series of new and polyfunctionalized triazolo[5,1-*b*]quinazolines and benzimidazo[2,1-*b*] quinazolines were synthesized. The significant advantages of the developed strategy involve the construction of the corresponding heterocycles by eliminating the use of precious catalysts under a mild condition in good yields.

Graphical Abstract:



Keywords:2-Aminobenzimidazole, Benzimidazo[2,1-b]quinazoline, Domino reaction, Potassium tert-butoxide, α–Tetralone, 1,2,4-Triazol-5-amine, Triazolo[5,1-b]quinazoline.

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Use of cyclic aliphatic ketones for spiro 2-amino-3-cyanopyrano[3,2-c]chromene formation.

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Abstract:

The three component reaction between 4- hydroxycoumarin, malononitrile and carbonyl compounds in ethanol in the presence of morpholine as a catalyst was studied. Only cyclic aliphatic ketones afford spiro 2-amino-3-cyanopyrano[3,2-*c*]chromene derivatives.

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Identification lncRNA-protein interaction pairs specific to Congenital Pouch

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Background: Congenital Pouch Colon CPC) is a rare genetic anorectal anomaly common to North Western India specifically Rajasthan. Since 2005 and aftermath of the human genome project, several efforts have been made to understand the rare variants and clinical genetic makeup of CPC, but no attempt on the identification of non-coding genes was made from whole exomes. We have earlier reported CPC's rare variants from whole exome sequencing across 18 affected in a total of 64 subjects. Recent reports show distinct mutational signatures in the form of non-coding RNAs as well, even as it remains to be understood if it is the advent of sequencing chemistry. We aimed to identify the long non-coding RNA (lncRNA) and protein interactions specific to this rare phenotype as congenital pouch colon anomaly from a whole exome sequencing sample. In this process, we have used a Smith-Waterman algorithm to detect lncRNAs from whole exome sequencing samples of CPC with predictions from the Noncode database. In this process, a couple of lncRNAs have been detected for which we screened identified and quantified using qPCR after raising primers. Further analyses include isolation of six proteins ranging between 33Kda to 156 Kda known to be interacting with one of the lncRNAs of interest. The *in-silico* predictions ascertaining the interactions between the small molecules have been confirmed using microscale thermophoresis (MST).

In this work, we report the identification of a lncRNA (NONHSAT008982) shown to be promiscuously interacting with a kinesin like proteins (KIF13A) and interleukin33 among the other four zinc finger, pikachurin, Pan-2 and butyrophilin precursor. With the discovery of 18 affected individuals via exome sequencing and further validation, these distinct mutational signatures notably are found in the form of lncRNA and the protein interaction pairs possibly define that exomes harbour non-coding mutational spectrum which serve as potential therapeutic targets.

Keywords: Congenital Pouch Colon, long non-coding RNA, *in-silico*, exome

P-346

Molecular docking and pharmacokinetic prediction of Thiazolidine-2,4-dione derivatives *in silico*.

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ABSTRACT

Background: Type 2 diabetes mellitus (T2DM) being a leading endocrine disorder has been a major public health issue that affects millions of people worldwide. With this chronic disease mainly characterized by high insulin resistance, the commonly prescribed oral therapeutic for type-2 diabetes mellitus are not so satisfactory and have varied limitations. Thiazolidine-2,4-diones(TZDs) are a class of oral hypoglycemic agents that act on Peroxisome proliferator activating receptor-γ (PPAR-γ) receptors and are mainly expressed in the adipose tissues. After binding with thiazolidine-2,4-diones, a conformational change occurs in the receptor which leads to sequence of steps ultimately activating the transcription of specific target genes. With PPAR-γ antagonists/agonists showing adverse side effects, there is a need to synthesize and develop newer drugs from these class of compounds

Objective : Virtually screen, dock, predict pharmacokinetic of Thiazolidine-2,4-dione derivatives and to further synthesize a cohort of them.

Methodology:- Molecular docking study on Thiazolidine-2,4-dione derivatives was performed using open source docking software keeping in view of the parameters like ADMET, bioactivity prediction and drug likeliness A careful representation using IUPAC nomenclature system was further ensued to virtually screen them for synthesis in the laboratory

Results and Discussions: The effects of newly designed analogues towards antidiabetic conditions along with possible receptor/ligand binding affinities were studied in silico. Also, we would like to predict their role towards endocrine disruption.

Future Perspectives: Once the analogues are designed in silico and chemically synthesized, further studies would be required to test their *in vitro and in vivo* efficacy either alone or in synergism with current drugs in use, as newer treatment strategy against diabetes.

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P-347

Acoustical studies of some novel chalcones in DMF and DMSO at different temperatures

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Abstract

Some novel chalcone derivatives have been synthesized and their structures were confirmed by spectroscopic techniques such as IR, NMR and mass. The density, viscosity and ultrasonic velocity of these chalcone derivatives have been measured in dimethyl sulfoxide and N, N-dimethylformamide at different temperatures over a wide range of concentrations. From these experimental data, various acoustical and apparent molar parameters were calculated. The results were interpreted in terms of solute–solvent and solute–solute interactions which gives idea about structure making or structure-breaking abilities of studied compounds in both solvents.

Keywords

Chalcone derivatives, ultrasonic velocity, density, viscosity, acoustical parameters, dimethylsulfoxide, N, N–dimethyl formamide.

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P-348

SYNTHESIS AND CHARACTERISATION OF 1-(SUBSTITUTED PHENYL)-2-(CYCLOHEXYLAMINO)-2-OXOETHYL 2(3,4DIFLUOROPHENYL) CYCLOPROPANE CARBOXYLATEDERIVATIVES VIA MULTICOMPONENT APPROACH

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Abstract: As per current research work, passerine reaction is an established efficient route for atom economy to synthesis pharmaceutically active component. So from sited a literature review on passerine reaction we reported here an efficient synthesis of 1-(*substituted phenyl*)-2-(*cyclohexylamino*)-2-oxoethyl-2-(3,4-*difluorophenyl*)cyclopropane carboxylatederivatives by using a simple and atom-economical pathway. A reaction of aldehyde with aromatic acid and isocyanide in the presence of MDC at room temperature by using multicomponent approach. The structures of newly synthesized compounds have been confirmed by their analytical and spectral (IR, ^{1}H NMR, ^{13}C NMR and mass) techniques.

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TOXIC AND NON-TOXIC PLANTS

Mayur A. Sonigara , Prakshal A. Gandhi and Tarun M. Patel

Abstract: The degree to which a substance (a toxin or poison) can harm humans or animals. Acute toxicity involves harmful effects in an organism through a single or short-term exposure. Subchronic toxicity is the ability of a toxic substance to cause effects for more than one year but less than the lifetime of the exposed organism. Non-toxic" is a marketing term used to describe many household cleaners. What exactly does it mean and is it protecting us? Should consumers trust the term or go further and check ingredients. Sago palm, tulips, azaleas, lilies…

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Synthesis of Silver Nanoparticles using Dimeric Gallate: Characterization and their antimicrobial efficacy

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The gallic acidis an abundantly available plant phenolic compound and a powerful antioxidant. In the present study we synthesized a dimeric analogue of gallic acid (DGA) and it was used to produce smaller sized **(~20 nm)**and stable silver nanoparticles (AgNPs)[1]. Different concentration of DGA were used ranging to reduce and simultaneously stabilize AgNPs. A typical surface plasmon resonance was observed at ~ 420 nm without any sign of aggregation. The antimicrobial potential of such AgNPs was evaluated in four different bacterial and fungal strains [2]. The nanoparticles showed efficacious bactericidal activity (~ 5 µg/ml) and fungicidal (~10µg/ml) activity against all the strains. The activity was also substantiated by means of optical and scanning electron microscopic studies. The significant antioxidant and antiplatelet activity of the nanoparticles represent them as suitable and versatile antimicrobial agents.The DGA could be an effective experimental candidate which would play an important role for the pertinent issue of scaling-up with lowvolume. Concisely, these DGA stabilized Ag nanoparticles could serve as promising antimicrobial agents for effective outcomes.

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P-351

Multi component approach toward pyrazolo[1,5-a]pyrimidine; Design, synthesis and characteristics studies

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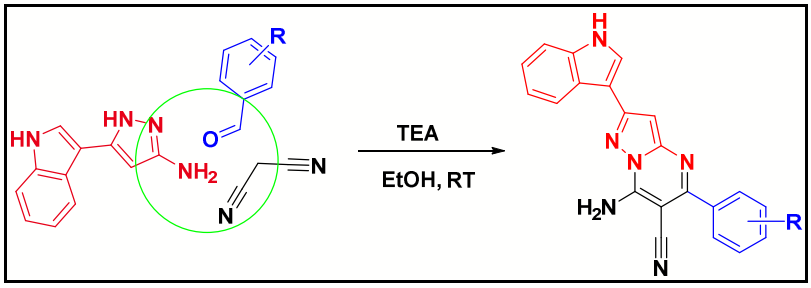
Abstract:

Nitrogen-containing heterocyclic compound great interest since they exhibit numerous biological activities. In present work, we have synthesisindole-basedpyrazolo[1,5-a]pyrimidin derivative viathree component one port reaction of5-(1H-indol-3-yl)-1H-pyrazol-3-aminewith malononitrile and various aromatic aldehyde. The significant advantage of the developed strategy involves mild basic, environmentally friendly condition and having a good yield at room temperature.

All the synthesized compounds are characterized by using various spectroscopic techniques like ^{1}H-NMR, ^{13}C-NMR, Mass and IR spectroscopy.



Keyword: pyrazolo[1,5-a]pyrimidin, three component one port condensation,mild basic condition, room temperature, domino reaction.

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P-352

Ultrasonic irradiation approaches to some new isooxazole bearing pyrazolo nucleous; Design, Synthesis and Characterization study

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Abstract:

Green chemistry is an environmentally benign chemistry. All Heterocyclic compounds have importants in medicinal chemistry. From literature survey it is found that isooxazole having some biological activity like antibacterial [1], anticholestermic[2],anthelmintic[3], Insecticidal [4] and antimicrobial [5] etc. In continuous present work we have synthesized a series of new (E)-4-((3-(substituted phenyl)-1-phenyl-1H-pyrazol-4 yl) methylene)-3-isopropylisoxazol-5(4H)-ones using hydroxylamine hydrochloride, aldehyde and using water as a solvent.
In present work we have developed greener route for the synthesis of proposed molecules by ultrasonic irradiation having shorter reaction time and minimizes the impurities formation. All the synthesized compounds were characterized by using various spectroscopic techniques like ^{1}H-NMR, ^{13}C-NMR, Infrared and mass spectroscopy. All spectral data give reliable results towards synthesis of targeted molecules.

Key-words: Ultrasonic irradiation, greener route, isooxazole bearing pyrazolo nucleous derivative.

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P-353

Microwave Assisted Cu(I)-CatalyzedHighly Efficient Approach for One-Pot Synthesis of Pyrazole Derivatives Using A^3 Coupling.

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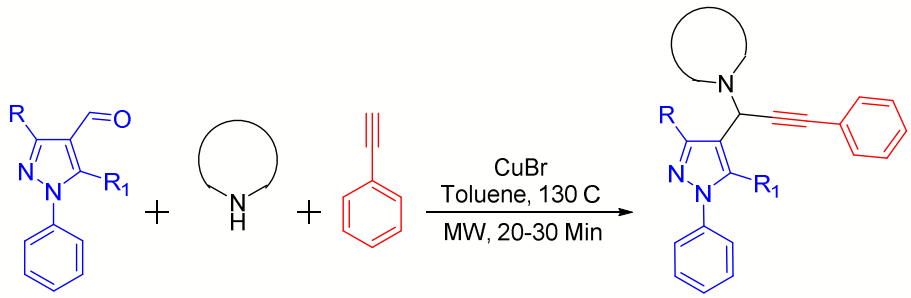
Abstract:

CuBr-catalyzed three component one-pot A3 coupling reactions were investigated under microwave irradiation.Although metal-catalyzed A3-coupling reactions have been extensively used to synthesize various propargylamine. Till A3 coupling is not tested in many heterocycles like substituted pyrazole.Pyrazole-4-carboxaldehydes, alkynes and amines with a variety of structures have been tested against Copper based catalyst. Best results achieved by Copper(I)bromide catalyst via microwave irradiation. Overall 15 subtracts of Pyrazole based propargylamine was synthesize . A catalyst loading of 20 mol% was sufficient to give excellent yields under microwave irradiation. In this study, set of reactions carried out under various Cu (I) and Cu (II) catalysts as well as different solvents and different stoichiometric ratio. This synthesis route made a great difference and resultant protocol was very convenient and excellent yielding for the generation of a broad substrateof heterocyclic substituted propargylamine.

Graphical Abstract:



Keywords: Pyrazole-4-carboxaldehydes, A3 coupling, Copper Catalyzed, Microwave Assisted

P-354

A review on Dendrimer: A novel functional molecule

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The research emphasis in dendrimer chemistry has recently switched to an exploration of the practical usefulness of functional dendritic molecules.Dendrimers, in contrast to linear polymers, are highly branched, fractal-like macromolecules of defined three-dimensional size, shape and topology which can be prepared with very narrow molecular weight distribution.

The term "functional dendrimer" is used to describe dendritic molecules which possess useful or reactive functional groups that can participate in chemical/physical processes without degrading the dendritic matrix.

This review summarizes the synthesis and its wide-ranging potential applications in many fields such as: healthcare, electronics, photonics, biotechnology, engineering products, pharmaceuticals, drug delivery, catalysis, electronic devices, environmental issues and nanotechnologies.[1,2] This is due to the ease of integration of these unique globular molecules with more mature areas of chemistry.

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P-355

A review on green syntheses of silver nanoparticles using plant extracts

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Kanoria Mahila P.G Mahavidhyalaya

Abstract

The Nobel metals like silver, gold, platinum, palladium, copper, zinc, and iron were usedin synthesis of particles of nano size. These nanoparticles are used in every phase of science along with engineering including medical fields and are still attracting the scientists to explore new dimensions for their respective worth which is generally attributed to their corresponding small sizes. The up-and-coming researches have proven their antimicrobial significance. Among several noble metal nanoparticles, silver nanoparticles have attained a special focus. Conventionally silver nanoparticles are synthesized by chemical method using chemicals as reducing agents which later on become accountable for various biological risks due to their general toxicity; engendering the serious concern to develop environment friendly processes. Thus, to solve the objective; biological approaches are coming up to fill the void; for instance green syntheses using biological molecules derived from plant sources in the form of extracts exhibiting superiority over chemical and/or biological methods. These plant based biological molecules undergo highly controlled assembly for making them suitable for the metal nanoparticle syntheses. The present review explores the huge plant diversity to be utilized towards rapid and single step protocol preparatory method with green principles over the conventional ones and describes the antimicrobial activities of silver nanoparticles.

Keywords: Plant extract, Green synthesis, Antimicrobial

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P-356

Study of nitrogen-heterocycles and pyrazolones as ligands and their complexation and pharmacological aspects

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Transition metals exhibit different oxidation states and are stabilized by chelating ligands. Nitrogen-heterocycles are important class of organic compounds having wide range of applications. An attempt was made to use pyrazolones as ligands and arecomplexed with some selective transition metals. More attention was made on copper complexes. Both ligands and complexes are characterized by elemental analysis, molecular weight determination and different spectral techniques (UV, IR, NMR). These were used for screening of antibacterial and antifungal activities against common standard strains like *E.coli, S.aureus, C.albicans* etc. Minimum Inhibitory Concentration (MIC) of complexes and ligands were assessed for above strains. Complexes were found to be more relevant for pharmacological and clinical applications.

Key Words : Transition Metals, Nitrogen-heterocycles, Pyrazolones, MICs, Biorelevant.

P-357

Synthesis and Structural Studies of some Cobalt Complexes containing derivatives of 8-Hydroxy Quinoline.

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Abstract: Ligands with *N, O*-chelation have well been studied. Of these, 8-Hyrdroxy Quinoline is extensively used as a versatile bi-dentate ligand in co-ordination chemistry [1]. It is a uni-negative ligand with alkoxy, and pyridine like donor groups. We are currently working on the synthesis and study of range of ligands containing one or more 8-hydroxy Quinoline units bridged through ether linkages of hydroxyl moiety. There are few such ligands, and their metal complexes have already been published [2]. Herein We report our preliminary result in this area with our studies on the synthesis, and crystals structures of cobalt complexes of three different types of ligands with different number of chelating groups, such as 1,3-bis(8-quinolyoxy)propane (**1**), a *N, O, O', N'* - tetradentate ligand, 8-(2-pyridylmethoxy)quinoline (**2**), a *N, O, N'* - tridentate ligand, and 8-methoxyquinoline (**3**), a *N, O* - biidentate ligand.

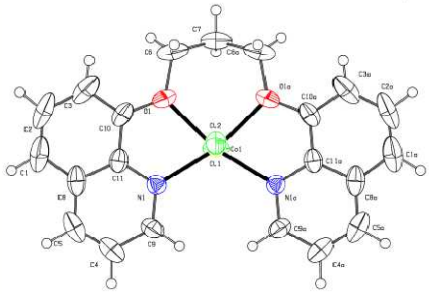

Figure 1: A prospective view of the structure of Cobalt complex (**4**) of 1,3-bis(8-quinolyoxy)propane, a *N, O, O', N'* - tetradentate ligand.

The Cobalt (II) chloride complex was prepared by reacting $CoCl_2.6H_2O$ with 1,3-bis(8-quinolyoxy)propane with a molar ratio of 1:1 in methanol at room temperature. Slow evaporation of an alcoholic solution of complex **4**afforded orange-red crystals suitable for X-ray.

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P-358

Metal-free, solvent depended regio- and stereoselective syntheses of allylic thioethers

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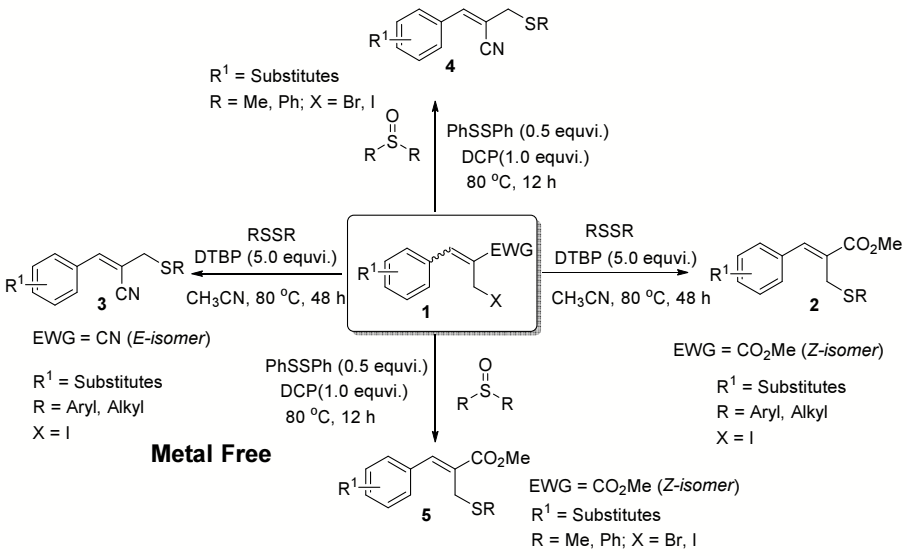
Abstract: Thioethers have been found to playing important roles in organic synthesis, the pharmaceutical industry, and materials science.[1] A solvent controlled, metal free, regio and stereoselective synthesis of allylic thioethers using allyl iodides/bromides and aryl or alkyl disulfides as coupling partner are described.[2] When the reaction carried out using DMSO/DPSO, the S-methylation/phenylation occurred whereas in CH_3CN the corresponding aryl/alkyl allyl thioethers were obtained. The densely functionalized allyl iodides/bromides[3] having different stereochemistry (E & Z) reacted well with a variety of disulfides in regio and stereoselective manner providing the resulting allyl thioethers in good to excellent yields.



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P-359

Triethanolamine catalyzed expeditious and greener synthesis of 2-amino-4*H*-chromenes

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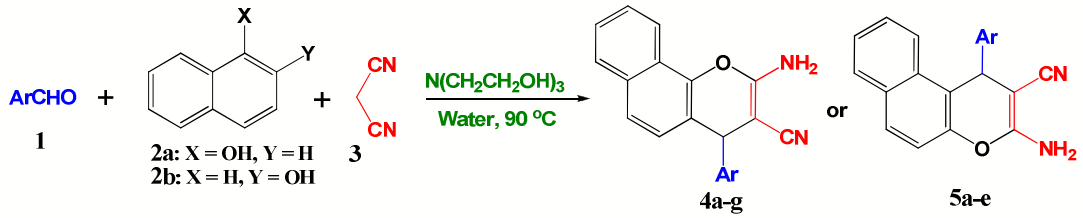
Abstract:
Triethanolamine (TEOA), an inexpensive and ecofriendly base, efficiently catalyzed three component condensation reaction of aromatic aldehyde, (□□□)-naphthol and malononitrile in water to give corresponding substituted 2-amino- 4*H*-chromene derivatives in excellent yields.

Keywords: Triethanolamine (TEOA), multi-component reaction, water media, 2-amino-4H-chromene, green synthesis

Graphical Abstract:



P-360

Design, synthesis and anticancer activity of β-carboline derivatives

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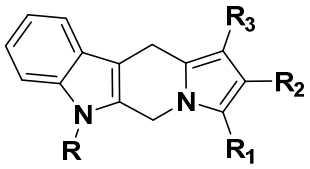
Abstract:

We have successfully applied bioisoster approach for the design and synthesis of new anticancer moleculesfromβ-carboline motif. The newly synthesized molecules weretested for their *in vitro* anticancer activity against various cancer cell growths. The most active compounds from the newly synthesized derivatives were tested for their *in vivo* as well as primary mechanistic study.We found that,these derivativesexhibits potent antitumor activity against CCRF-CEM, PC3, H1299 & OECM1 solid tumour growths. The most potent derivatives were further screened for in vivo study using xenograft model. Primary mechanistic study revealed that they exhibit anticancer effect through DNA cross linking & Topoisomerase inhibition.

Keywords:β-carboline, bioisoster, anticancer activity, DNA cross linking, Topoisomeraseinhibition

Graphical Abstract:



P-361

Microwave assisted, facile and generalized synthetic protocol for preparation of benzimidazole derivatives

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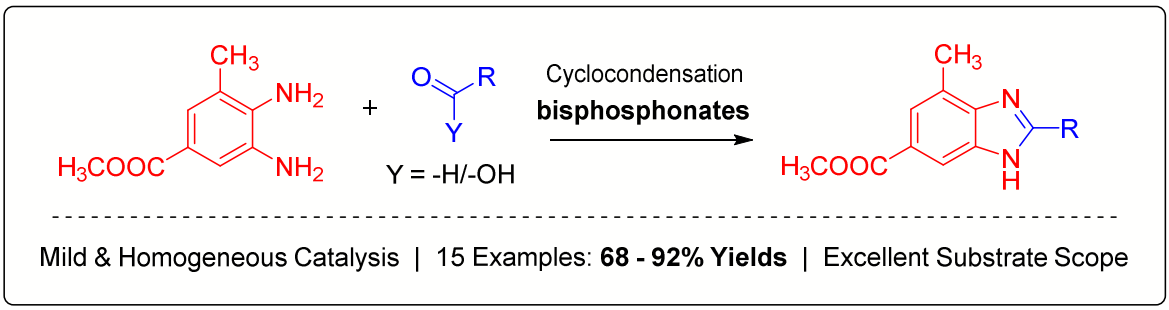
Abstract

A facile and efficient cyclocondensation reaction of substituted *o*-phenylenediamines with an aldehyde or carboxylic acid using bisphosphonates to furnish hitherto unreported Methyl 4-methyl-2-substituted-1*H*-benzo[*d*]imidazole-6-carboxylatederivatives is described. A new and efficient protocol was developed as a homogenous catalyst for the synthesis of benzimidazoles under conventional and microwave irradiated reaction atmosphere. This methodology has the advantage of excellent yields with short reaction time and highly robust & practical reaction arrangement.

Keywords

Homogenous catalyst, bisphosphonate, microwave assisted organic synthesis (MAOS), benzimidazoles, fused heterocycles, cyclocondensation.

Graphical Abstract



P-362

Transition metal free C(sp^3)-H sulfenylation of 2-aminopyridinium ylide: Synthesis of 2-hydroxy-3-sulfenylimidazo[1,2-*a*]pyridines

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The high importance of nitrogen-containing compounds in the realm of natural products, biological systems and organometallics has sparked significant research efforts for their efficient synthesis. In this disciple, imidazo[1,2-*a*]pyridine scaffold is known as privileged structure with an extensive range of biological activities such as antiviral, antibacterial, fungicidal, and anti-inflammatory properties [1]. These molecules are also the core structure of many commercially available drugs such as Alpidem, Zolpidem, Zolimidin, Olprinone, and GSK-812397. The ubiquitous emergence of such compounds in the pharmaceutical industry resulted in an ever-growing interest in the synthesis of C-3 and C-2 functionalized imidazo[1,2-*a*]pyridines [2]. Among numerous heterocyclic compounds, sulfur containing heterocycles also are important auxiliary units in numerous naturally occurring and bioactive compounds. In recent years, sulfenylation of heterocyclic compounds has emerged as intriguing strategy for the synthesis of biologically active molecules. In this regards, the sulfenylation of imidazo[1,2-*a*]pyridine has been well established in the literature by various research groups [3]. In general, the existing methods rely on direct chalcogenylation of preexistingimidazo[1,2-*a*]pyridinering with sulfenylating agents such as sulfonyl chlorides, sulfonyl hydrazines or *S*-phenyl benzenesulfonothioate, disulfides however, synthesis of imidazo[1,2-*a*]pyridine and sulfenylation in one-pot are rare. In continuation to our effort towards synthesis of functionalizedimidazo[1,2-*a*]pyridine from pyridiniumylide [4], hereinwe will present a poster, demonstrating the synthesis of 2-hydroxy-3-sulfenyl imidazo[1,2-*a*]pyridine*via*transition metal free C(sp^3)-H sulfenylation of 2-aminopyridinium ylide.

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P-363

Synthesis of Hydroxamic Acidsusing ImidazoliumSalt Supported *N*-HydroxySulfonamide as Soluble Support

Saroj, Khima Pandey and Anil Kumar*

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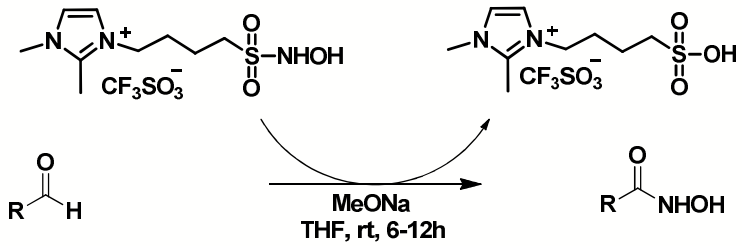
Abstract

Hydroxamic acids are a privileged class of compounds with potent and a broad array of biological activities, such as antibacterial, antifungal, anti-inflammatry, anti-asthmatic properties[1]. The hydroxamic acid funcationality is present in several natural products, drugs(e.g. Vorinostat) and in metal ion chelators [2]. Hydroxamic acids are generally synthesized from activated carboxylic acids (esters, anhydrides and acid chlorides etc.) and protected/unprotected hydroxyl amines.AngeliRemini reaction is an interesting method for the synthesis of hydroxamic acid from aldehyde using *N*-hydroxybenzenesulphonamide [3]. However, these methods suffer from some disadvantages such as requirementof protection and deprotection of hydroxyl amine, preparation of special linker (solid phase synthesis), removal of side product and product purification.

With increasing importance of hydroxamic acids in drug design as well as in organic synthesis and our interest exploring application of ionic liquids in organic synthesis we have developed an efficient method for the synthesis of hydroxamic acids from aldehydes using imidazolium supported *N*-hydroxysulphonamide (Scheme 1).Homogeneous reaction conditions, high yields, easy removal of side product, chromatographic free purification are thesilent features of this approach.



Scheme 1: Synthesis of hydroxamic acids

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P-364

One-Pot Sequential Knoevenagel Condensation Followed by Pd(II)- catalyzed Intramolecular Oxidative C(sp^2)–H/C(sp^2)–H Cross Coupling Reactions: Direct Access to Annulated Indole Fused Aza-heterocycles

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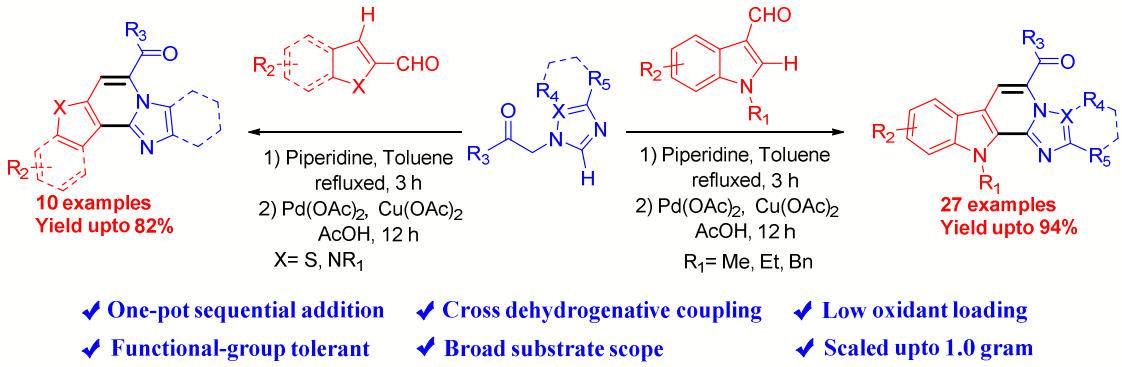
Transition metal catalyzed oxidative C–C bond formationhas been successfully exploited in recent era owing to their step and atom economy feature, however, the construction of targeted C–C bond is quite difficult to access fused aza-heterocycles. Usage of unfunctionalized starting material makes this strategy more environmental-friendly as compared to established cross coupling reactions, also a challenging task before the organic chemist. [1].

Among fused azaheterocycles, indole fused scaffoldhas rich chemistry and they are widely distributed in variety of natural products, synthetic molecules with diverse pharmaceutical properties[2].In view of their importance and our ongoing interest to develop new routes for the synthesis of aza-fused heterocycles[3]. Herein, we wish to report an efficient protocol forsynthesis of indole annulated *N*-heteroarenes in one-pot sequential Knoevenagel type condensation followed byPd(II)-catalyzed intramolecular oxidative C(sp^2)–H/C(sp^2)–H cross coupling fromactivemethylene azoles and*N*-substituted-1*H*-indole-3-carboxaldehydes (Scheme 1).



Scheme 1

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P-365

Rationale design and synthesis of some novel imidazole linked thiazolidinone hybrid molecules as DNA minor groove binders.

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Abstract

A novel series of imidazole linked thiazolidinone hybrid molecules were designed and synthesized through a feasible three step reaction protocol. The synthesized molecules were characterized by FT-IR, 1H NMR, 13C NMR and HRMS techniques. *In vitro* susceptibility tests against some gram positive (*Staphylococcus aureus, Bacillus subtilis)* and gram negative bacteria *(Escherichia coli* and *Pseudomonas aeruginosa)* showed broad spectrum potency of the molecules. The most active molecule (S2A7) gave MIC value of 2.0 µg/mL which is at par with the reference drug Streptomycin. Structure activity relationships revealed nitro and chloro groups are crucial for bioactivity if present at meta position of arylidene ring in 3-(3-(imidazol-1-yl)propyl)-5-(benzylidene)-2-(phenylimino)thiazolidin-4-one. DNA and BSA binding studies of S2A7 under simulated physiological pH were probed with UV-Vis., fluorescence quenching, gel electrophoresis and molecular docking techniques. These studies established that S2A7 has strong affinity towards DNA and binds at the minor groove of DNA with binding constant (Kb) of 0.1287 x 102 L mol-1. Molecular docking simulations predicted binding affinity of -9.2 & -7.2 kcal/mol respectively with DNA & BSA. Van der Waals forces and hydrogen bonding interactions were predicted as the main forces of interaction. In case of DNA S2A7 exhibited specific affinity towards adenine-thiamine base pairs. The compound forms a stable complex with BSA by binding at subdomain IIIA indicating high biodistribution.

P-366

Salix Caprea: Isolation, Simultaneous quantification, method validation of five polar Secondary metabolites by LC/MS.

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Abstract

Twelve constituents were isolated and identified from medicinally important plant *Salix caprea*, among these four were flavonoids, three were steroids, four were fatty acids and one was sugar. One constituent selected from each group was screened for in vitro immunomodulatory potential employing Con A (40µg/well) to stimulate T-cells or LPS (40µg/well) to stimulate B- cells proliferation of Mice Splenocytes *by* MTT assay. A rapid, precise, sensitive and validated LC/MS method for simultaneous quantification of 5 polar constituents (MA, RU, LG, QU, KA) was developed. Formic acid was 0.1% in water showed complete separation. The method was validated for accuracy, precision, LOD, LOQ and all calibration curves showed a good linear relationship ($r > 0.9956$) within test range, accuracy validation recovery 94.53–99.10% with RSDs <2.00%. Rutin (RU) was found major component (1056ng/mg) and mannitol (MA) the least (16.23ng/mg) in chloroform extract of inflorescence. Among all tested constituents, Kaempferol (K) showed maximum potential for suppression of CON-A stimulated splenocytes (ranging 68-87% of activity) in dose dependent manner at the conc. (10^{-6} to 10^{4}) whereas mannitol at low concentration suppressed LPS stimulated splenocytes above 43%. β-sitosterol showed least potential (6-8%). These natural products demonstrated a significant modulation against splenocytes proliferation.

Keywords: *Salix Caprea*, LC/MS, Secondary Metabolites, Immunomodulatory;

P-367

Isolation and identification of some biologically active compounds from three Indigenous *Cordia* species byTLC- UV absorption densitometry method

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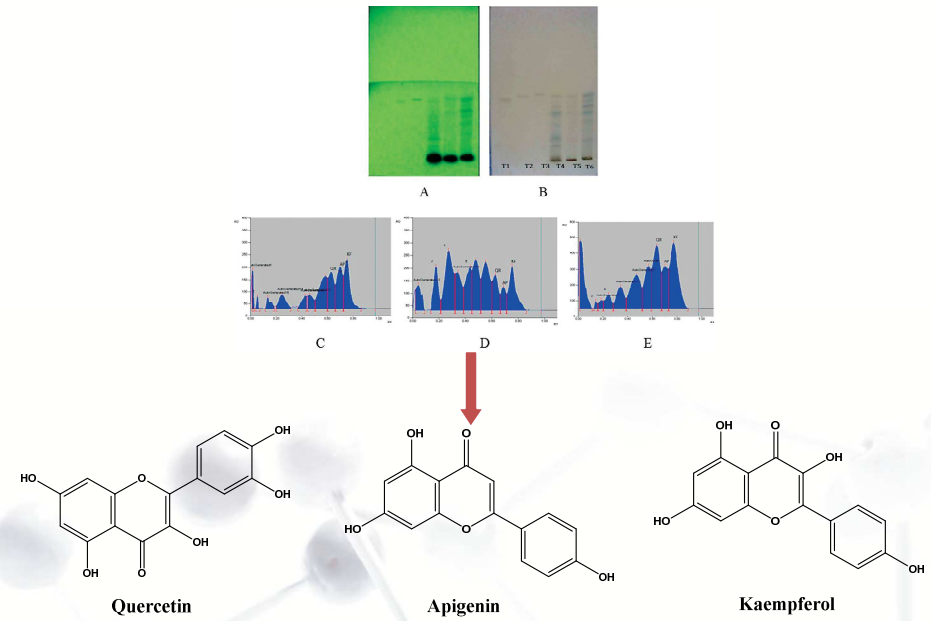
Abstract:

A following method involving toisolate and identify three biologically active flavonoids, quercetin, kaempferol, and apigenin, from the hydrolyzed methanolic extract of three indigenous *Cordia* speciesbarks using preparative thin-layer chromatography (PTLC) and high-performance (HP)TLC methods using reference standard. For achieving good separation, a mobile phase of toluene–ethyl acetate–GAA–formic acid (5:5:0.5:1) was used. The ultraviolet (UV)-based densitometry determination was carried out at 254 nm in reflection–absorption mode. The antioxidant compounds in the samples were screened through DPPH derivatization method. The methodwas partially validated in terms of linearity, specificity, and sensitivity. From this, it is concluded that planar chromatographyhas a potential as a rapid and simple tool for the identification and quantification of phytochemical in complex mixtures samples.

Keywords: Cordia, HPTLC, Quercetin, Kaempferol, Apigenin

Graphical Abstract



P-368

A facile synthesis of highly functionalized pyrazolo[1,5-a]pyrimidines using oxoketenedithioacetals as a synthon

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[b] *Department of Chemistry, Saurashtra University, Rajkot 360005, Gujarat, India*
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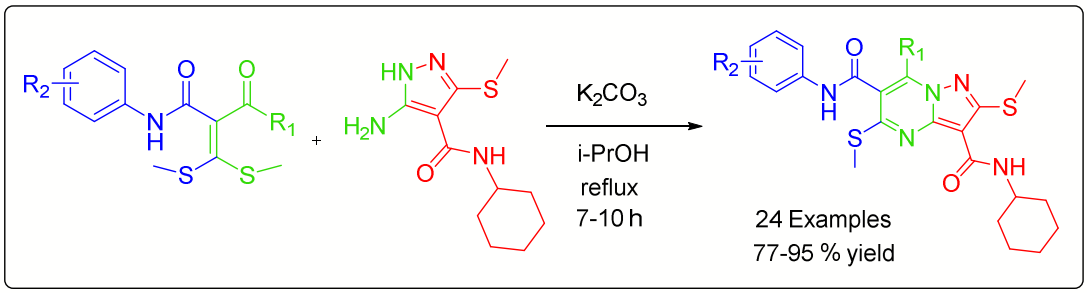
Abstract

Herein we report an effective strategy for the synthesis of highly functionalized pyrazolo[1,5-a]pyrimidines. A versatile type of synthon, oxoketenedithioacetals, react with 5-amino-*N*-cyclohexyl-3-(methylthio)-1H-pyrazole-4-carboxamide under variety of reaction conditions to afford highly functionalized pyrazolo[1,5-a]pyrimidines *via* [3+3] hetroaromatization. The results of the study described a simple approach for the synthesis of pyrazolo[1,5-*a*]pyrimidines with excellent yield and short reaction time using potassium carbonate base and isopropanol as a solvent.

Keywords

Heterocycles, Pyrazolo[1,5-*a*]pyrimidines, Heteroaromatization, Oxoketenedithioacetals, Cyclization

Graphical Abstract



P-369

Synthetic Approach for Various Potential pharmaceuticals based on 1,2,3-triazoles Heterocyclic Scaffolds via click chemistry approach

Y. B. Dudhagara[a], M. V. Parsania[b]

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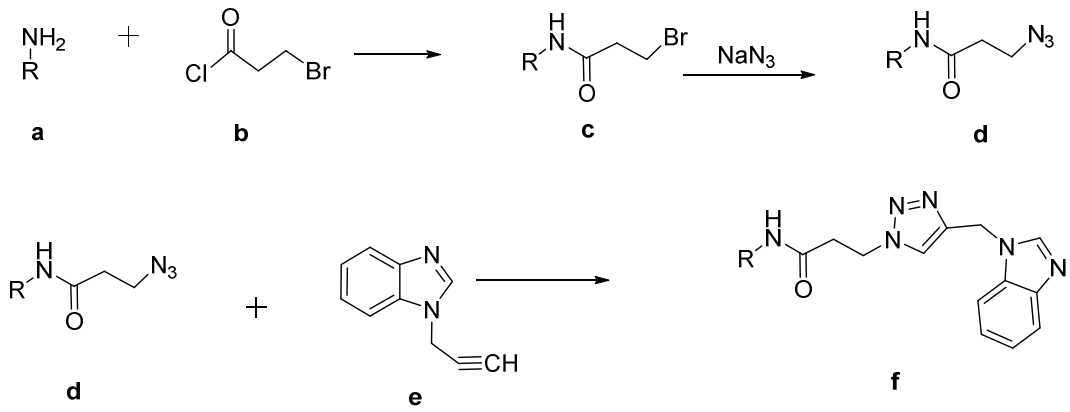
Keywords: 1-(prop-2-yn-1-yl)-1H-benzo[d]imidazole, 1,3-dipolar cycloaddition, 3-bromo-N-phenylpropanamide, click chemistry

Abstract.

Synthesis of new 3-(4-((1H-benzo[d]imidazol-1-yl) methyl)-1H-1,2,3-triazol-1-yl)-N-phenylpropanamide derivatives have been synthesized and studied with a view to understand and establish the effect of molecular structure on antifungal and antibacterial activity. Using 1,3-dipolar cycloaddition (click chemistry) reaction of 3-bromo-N-phenylpropanamide derivatives with 1-(prop-2-yn-1-yl)-1H-benzo[d]imidazole in the presence of Cu(I) catalyst has been achieved in very high yield Analytical and spectral data confirms the molecular structures.

Graphical Abstract:



P-370

SYNTHESIS AND CHARACTERIZATION OF SOME 3-(2-(5-PHENYL-1H-1,2,3-TRIAZOL-1-YL)ACETYL)-2HCHROMEN-2-ONES, USING CLICK REACTION

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[3] *Matushri Virbaima Mahila Science & Home Science College, Rajkot-36005*
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Abstract: Novel 1,2,3-triazoles were synthesised using the one-pot reaction of, 3-(2-azidoacetyl)-2H-chromen-2-one and terminal alkynes in the presence of water: t-BuOH: DMF(1:1:1) using the click approach, The new therapeutically active 1,2,3, triazole compounds have been synthesized bearing coumarin moiety The structures of compounds have been confirmed by various spectroscopic methods.

Keywords: Coumarin, 1,2,3-triazoles, Click chemistry

P-371

A novel luminescence probe based on Schiff base for Al^{3+} ions

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Abstract: In this study, two new Schiff base receptors 2-((*E*)-(3-((*E*)-2-hydroxybenzylideneamino)phenylimino)methyl) phenol **(R1)** and 2-((*E*)-(2-((*E*)-2-hydroxybenzylideneamino)phenylimino)methyl)phenol **(R2)** have been fabricated and characterized by several instrumental analytical techniques *viz.* CHNS analyzer, FT-IR, HRMS and ^{1}H-NMR spectroscopic techniques. The developed sensor can be employed as naked-eye "ON-OFF" type luminescent sensor for detection of Al^{3+} ions and the detection can be usage by the considerable color changes from colorless to sharp bright blue under UV light in methanolic solution. The receptors show large luminescence enrichment upon addition of Al^{3+} ions which is distinguished by colorimetry. In addition to this, the stability constant and the limit of detection of the receptor–Al^{3+} complexes were also calculated via the luminescence titration method. The developed receptors work significantly in the pH range of 6–8. Thus, the developed receptors could be utilized for the assessment of Al^{3+} ions qualitative as well as quantitative in solution. On the other hand, the decrease in HOMO-LUMO band gap energy confirmed the more binding ability of receptors with Al^{3+} ions. Thus the receptor can be used to estimate Al^{3+} ions in the presence of (Ba^{2+}, Ca^{2+}, Cs^{+}, Cr^{3+}, Fe^{2+}, Fe^{3+}, Li^{+}, Na^{+}, K^{+}, Mg^{2+}, Mn^{2+}, Nd^{3+}, Pb^{2+}, Co^{2+}, Cd^{2+}, Gd^{3+}, Hg^{2+}, Cu^{2+}, Zn^{2+}, Ni^{2+} and Sr^{2+}) other metal ions. Subsequently, it is of immense utility for analyse huge number of analytical, biological and environmental samples.

Keywords: Luminescence, Colorimetry, Schiff base, Receptor

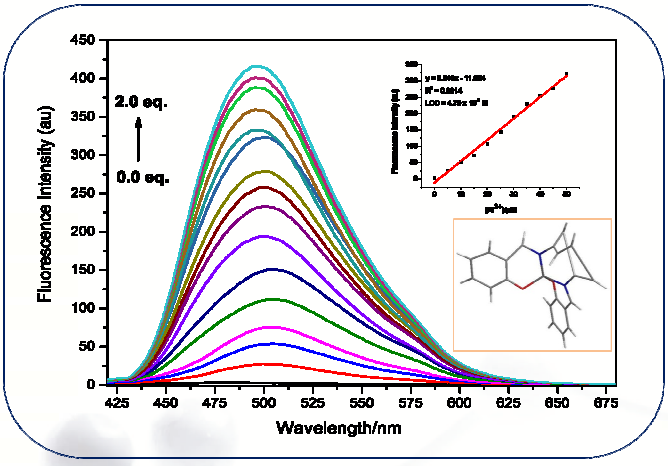

Figure: Changes in the luminescence spectra of receptor **R1** with externally added [Al^{3+}] ions. [Al^{3+}] = 0.0–500 µM, (from bottom to top). Inset: linear plot between added amounts of metal ion (0.0-50 µM) top and structure of **R1** bottom).

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P-372

Oxidant-Controlled C-sp2/sp3 – H Crossdehydrogenative Coupling of *N*-Heterocycles with Benzylamines

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In recent years, oxidative cross coupling reaction has gained a tremendous importance in synthetic organic chemistry.[1,2] Organic transformations for direct conversion of C-H bonds to C-C bonds is a hot area in organic chemistry because they are atom economical and provide short route for construction of C-C bonds.[3,4] Formation of C-C bonds from two different C-H bonds is known as 'cross dehydrogenative coupling (CDC)' reaction and it does not require pre-functionalized starting materials.[5,6] In this context, the activation of C-H bonds (sp2, sp3) remains a challenging task for synthetic organic chemists.[7,8] We devolped ionic liquid mediated cross-dehydrogenative coupling (CDC) of benzylamines with *N*-heterocycles having sp2 or sp3 carbon which results in the formation of *C*-benzoylated or alkenylated products. Benzoylation of *N*-heterocycles occurs via (NH4)2S2O8 catalyzed benzoyl radical formation. An oxidative alkenylation of *N*-heterocycles having *C*-sp3 carbon (2-methylazaarenes) occurs via deamination of benzylamine followed by Csp3-H bond activation in high stereoselectivity. Both benzoylation and alkenylation protocols are metal-free, green, simple, efficient and tolerates wide variety of functional groups.

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P-373

A Theoretical Study of Dye-SensitizedSolar Cell:Density Functional Theory Based Approach

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In modern days, solar cells have gained a lot of importance in view of its environment-friendly and sustainable behaviour. Due tomany fold applications, Dyes Sensitized Solar Cells (DSSCs) have become popular among all other solar cells. Experimental and theoretical studies are being carried out to explore different aspects of DSSCs. Density Functional Theory (DFT) has emerged as important theoretical approach to provide an insight aboutactivities and properties of DSSCs.

Recently, we have proposed a new scale of electrophilicity index (ω), aDFT based conceptual descriptor, in terms of empirical approach. Electrophilicity indices of 103 elements of the periodic table have been computed in force unit. The concept is conceived considering electrophilicity index of an atom as a function of attraction between nuclear and valence electron. We have also successfully established electrophilicity equalization principle of certain molecular species using of our computed atomic data.

In this venture, we have correlated the experimental results of mono and bi-anchoring metal-free organic dyes, containing diphenylamine or dimethylamine,in terms of our computed molecular electrophilicty indices. A close agreement between our computed data and experimental data establishes efficacy of our model. Our computation has inherent significance due to its economic sustainability.

Key words: Dyes sensitized solar cells, DFT, Electrophilicity index, Force concept

P-374

Palladium-catalyzed aminocarbonylation of halo-substituted 7-azaindoles and other heteroarenes using chloroform as a carbon monoxide source

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A palladium-catalyzed aminocarbonylation of halo-substituted 7-azaindoles utilizing $CHCl_3$ as the carbonyl source has been developed for a straightforward incorporation of amide functional group. The protocol was extended to other heteroarenes such as pyrazolopyridines and indazoles. The substrate scope of the reaction with respect to heteroarenes and the amine component is reported. This method offers an alternative avenue for aminocarbonylation of pharmaceutically important hetero-cycles.

Azaindoles are a privileged heterocyclic cores exhibiting significant biological activities and are utilized as pharmacophores in drug discovery programs.[1] The presence of two neighbouring nitrogen atoms in a 7-azaindole system, the bioisostere of indole or purine base, due to their neighbouring hydrogen-bond donor and acceptor properties, have been explored extensively for various therapeutic indications.[2] Two drugs named Vemurafenib and Venetoclax, containing a 7-azaindole core, recently gained FDA approval, and several other 7-azaindole-containing drugs are in various stages of clinical development.[3] Due to their therapeutic importance, methods for the synthesis and functionalization of azaindole and derivatives have attracted considerable interest.[4] A particularly interesting subset of these molecules are therapeuticaly promising amide-substituted derivatives (Figure 1).[5] While amide bond formation *via* transition-metal catalyzed direct aminocarbonylation are reported for indole systems,[6] amide bond formation with an azaindole moiety have only been reported in a traditional way.[7]

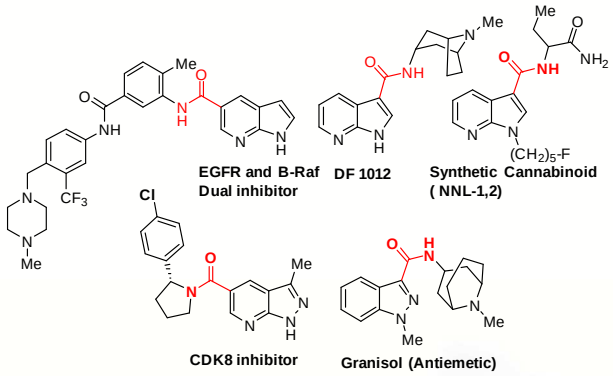
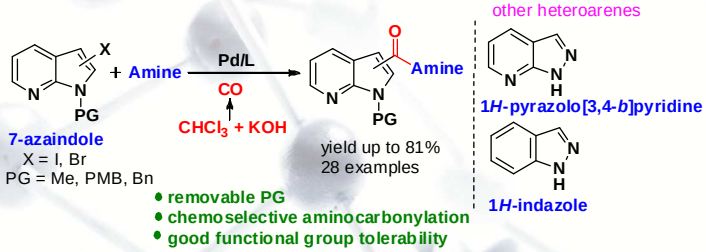


Fig. 1 Biologically active 7-azaindole with amide group



Scheme 1 Aminocarbonylation of **halo-substituted** 7-azaindoles and other hetero arenes

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P-375

Nanocatalytic practices: An Environmentally benign Sustainable tactic to construct 3-substituted indoles

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Cu doped ZnS NPs nanoparticles were prepared by co-precipitation method and characterized by XRD, TEM, EDAX, ICP-AES, and UV–vis analysis. The results showed that these particles have an average size of approximately 4–5 nm. The synthesized nanocatalyst was utilized for its catalytic applications towards the 'on water' one-pot synthesis of 3-substituted indoles *via* Knoevenagel/Michael addition reaction of indane-1, 3-dione, aromatic aldehydes and indole. The enhanced catalytic activity of ZnS NPs by Cu doping could be attributed to the increase of surface acidity. Further, the nanocatalysts were reused five times without significant loss of their catalytic activity in the same medium. The combination of these well-established approaches leads to the development of effective, rapid, and environmentally benign synthetic method.

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P-376

Insilico Design and Synthesis of Benzimidazole Derivatives as Anti-cancer Agents by Liquid Phase Combinatorial approach

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Nirma University

Due to the importance of benzimidazole moiety and its derivatives several been investigating various compounds bearing single substituents or substituents in heterocyclic ring system mainly inin 3rd,4th,and7thposition of ring system. Encouraged by the above observations we firstly carried out the 3D different benzimidazole bearing substituents acting on prostate cancer DU-145 cell line. From the 3D QSAR studiesit was found that the compound (2) was found to be most potent with low IC_{50} value. So we designed molecule on the basis of 3D QSARstudies.Then after designing of the molecules we performed docking studies of various molecules on topoisomerase enzyme form the studies using SYBYL X it was foundthat the compound MR6 and MR7 showed maximum interaction with the amino acids present over enzyme structure. After docking studies we designed synthetic scheme for synthesizing library of compounds using liquid phase technique. Then we carried out synthesis of different benzimidazole derivatives bearing amines and acids as changing substituents using liquid phase synthetic technique.

The synthetic protocol included 6 steps to synthesize the target molecules. First step is for synthesis is done using steglich esterification method to synthesis PEG tagged methyl ester benzoate from crude compound 4 fluoro 3 nitro benzoic acid. In the second step halo- amine replacement reaction takes place. In third step reduction of nitro group to amine occurs using Ammonium chloride and activated zinc. The fourth step includes formation of amide linkage using steglich process for amide formation. The fifth step includes ring closure to form core benzimidazole moiety along with different substituents. The characterization of the synthesized compounds were carried out using FT-IR, Mass and NMR spectroscopy.

Thus designing of the molecules was carried out on the basis of 3D QSAR results in which steric, electrosteric, hydrophobic, hydrogen bond acceptor and hydrogen bond donor etc region were obtained. By docking studies molecules compound (code: MR6, MR7) i.e containing nitro group.hydroxyl group gave maximum interactions with high scores. Synthesis of targeted compound was done using 6 steps which involved estcrification, halo-amine condensation, reduction of nitro compounds, amide bond formation and finally ring closure. After synthesis all the compounds were confirmed by analytical technique like IR, Mass spectroscopy etc. Thus it can he concluded that these synthesized molecules can act as potential inhibitors of topoisomerase enzyme.

P-377

Design, synthesis and antimicrobial activity of novel 1,3,4-oxadiazoles incorporating pyrazole scaffolds

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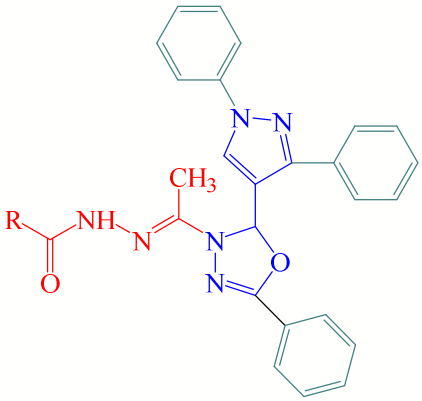
In search of new antimicrobial agents with improve potency, we have synthesized *N'*-(1-(2-(1,3-diphenyl-1-*H*-pyrazole-4-yl)-5-phenyl-1,3,4-oxadiazole-3(2*H*)-yl)ethylidene)-(aryl)-benzohydrazidesby combining 1,3,4-oxadiazole and pyrazole scaffolds having diverse pharmacological activities. All the newly synthesized compounds werecharacterized by different analytical techniques like IR, ^{1}H and ^{13}C NMR and mass spectrometry. These compounds have been evaluated for their *in vitro* antimicrobial activity against bacterial strains like*Staphylococcus aureus* (MTCC 96), *Streptococcus pyogenes* (MTCC 442), *Escherichia coli*(MTCC 443),*Pseudomonas aeruginosa* (MTCC 1688) and fungal strains like*Candida albicans* (MTCC 227), *Aspergillus niger* (MTCC 282) and *Aspergillus clavatus* (MTCC 1323) using serial broth dilution method. From the results, it was found that compounds with electron withdrawing groups showed excellent antibacterial activity while compounds with electron donating group showed very good antifungal activity.



P-378

Studies on bioactive heterocyclic compounds containing 1,3,4-oxadiazole moietyand their antimicrobial activity

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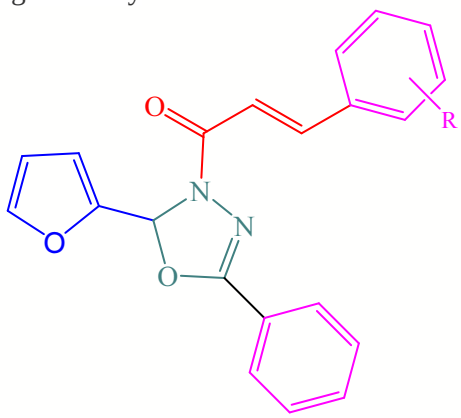
In a search of novel fused heterocycleshaving high activity and withlow toxicity, a series of compounds containing furan and 1,3,4-oxadiazole rings were designed and synthesized by a three-step synthetic route starting from furan-2-carbaldehyde and benzohydrazide. The structures of all the synthesized compounds were confirmed by ^{1}H NMR, ^{13}C NMR,mass spectrometry and elemental analysis. All the synthesized compounds have been evaluated for their *in vitro* antimicrobial activity against four bacterial strains*Staphylococcus aureus* (MTCC 96),*Streptococcus pyogenes* (MTCC 442), *Escherichia coli* (MTCC 443),*Pseudomonas aeruginosa* (MTCC 1688), fungal strainslike *Candida albicans* (MTCC 227), *Aspergillusniger* (MTCC 282) and *Aspergillusclavatus* (MTCC 1323) using serial broth dilution method. From the results, it was found that compounds with electron withdrawing group exhibited excellent antibacterial activity while compounds with electron donating group showed very good antifungal activity.



P-379

Synthesis on heterocyclic compounds and studies of their antimicrobial activity

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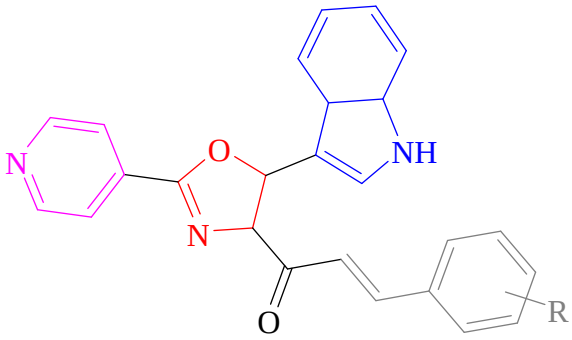
1,3,4-oxadiazole heterocycles are very good bioisosteres of amides and esters, which can contribute substantially in enhancing pharmacological activity by participating in hydrogen bonding interactions with the receptors. A series of twentynew pyridine containing 1,3,4-oxadiazole heterocycles were synthesized and characterized by analytical techniques like ^{1}H NMR,^{13}C NMR, IR and Mass spectrometry.The synthesized compounds were screened for their antimicrobial activity by serial broth dilution method.These compounds have been evaluated for their *in vitro* antimicrobial activity against bacterial strains *Staphylococcus aureus* (MTCC 96), *Streptococcus pyogenes* (MTCC 442), *Escherichia coli* (MTCC 443),*Pseudomonas aeruginosa* (MTCC 1688) and fungal strains*Candida albicans* (MTCC 227), *Aspergillusniger* (MTCC 282) and *Aspergillusclavatus* (MTCC 1323). From the results, compounds with electron withdrawing group found to possess excellent antibacterial activity.



P-380

Synthesis and antimicrobial screenig of 1,3,4 – oxadiazole derivatives

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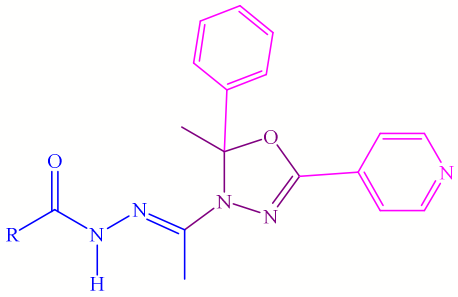
A series of novel 1,3, 4-oxadiazole derivatives were efficiently synthesized and characterized by IR, ^{1}H NMR, ^{13}C NMR spectroscopy and mass spectrometry. The newly synthesized N'-(1-(2-methyl-2-phenyl-5-(pyridin-4-yl)-1,3,4-oxadiazol-3(2*H*)-yl)ethylidene)benzohydrazides were evaluated for their *in vitro* antimicrobial activity against four bacterialstains like*Staphylococcus aureus*(MTCC-96), *Streptococcus pyogenes*(MTCC-442), *Escherichia coli*(MTCC-443), *Pseudomonas aeruginosa*(MTCC-1688, and three fungal*Candida albicans*(MTCC 227), *Aspergillusniger*(MTCC 282), *A. clavatus*(MTCC 1323)by using conventional broth micro dilution method.We observed that the presence of electron withdrawing groups at para position of phenyl ring enormously enhanced the antibacterial activity. From the results, they were found to possess excellent antimicrobial activity.The antimicrobial screening data revealed that selected screened compounds exhibited significant activity against all microbial and fungal strains.



P-381

Synthesis and characterization of heterometallic 3*d*-4*f* Polyoxometalates containing Silicotungstate

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Polyoxometalates (POMs) are an environment friendly self-assembled metal-oxygen nanocluster anions containing early transition metals (Mo, W, V, Nb and Ta) and a p-block element such as P, As, Sb, Bi, Si, Ge in their high oxidation state. They exhibit a wide range of structural diversityand reactivity.[1]Due to the intrinsic properties of POMs such as redox behavior, large sizes, high negative charges, nucleophilicity, they possess vast applications in the field of bio-fuels, bio-metallic catalysis, energy source (flow battery), single molecular magnets,etc.[3] The most fascinating aspect of POM is the self-assembly process leading to aggregates, which can be further linked in different ways. This self-assembled molecules generate nano-sizedmolecular materials with well-defined properties.

A series of heterometallic 3*d*-4*f* silicotungstates have been synthesized in a one-step reaction procedure on reacting withKeggin type trilacunary$Na_{10}[SiW_9O_{34}].23H_2O$precursor with $Ln(NO_3)_3.nH_2O$ where Ln = Pr^{III}, Nd^{III}, Sm^{III}, Eu^{III}, Gd^{III}, Tb^{III}, Dy^{III}, Ho^{III}, Er^{III}, Tm^{III}, and $Yb^{III}$and $CoCl_2.6H_2O$ in an aqueous potassium chloride solution. The synthetic procedure was followed similar to that of the previously reported paper containing keggin type phospho and silicotungstates but in the absence of any organic ligand.[2] The compounds formed were all potassium salts and were characterized by Fourier transform infrared spectroscopy (FT-IR), Single Crystal X-ray diffraction, UV-Visible spectroscopy.The crystal structure composed of three packman-shaped asymmetric entities and crystallized in triclinic crystal system having P-1 space group.The synthesis of these heterometallic polyoxometalates were done in an environment friendly way,in an open air syntheticprocedure.

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P-382

AN ALTERNATIVE APPROACH FOR COMPUTATION OF HALF WAVE POTENTIAL

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Abstract

Half-wave potential ($E_{1/2}$) has emerged as an important parameter to explain the redox processes and has gained a lot of significance. Half-wave potential is defined as a potential at which polarographic wave current equalizes to one half of the diffusion current. The half-wave potential can provide an insight for the study of complex chemical equilibria where experimental determinations are difficult. In this venture we have tried to define half-wave potential in an alternative simple approach, in terms of quantum chemical index, *viz*. Electrophilicity Index (ω). As this reactivity index deals with the electronic arrangement and nature of the atom/ molecule, it serves as a crucial quantity in the providing information regarding functioning of biological systems and redox processes. Recently, we have empirically computed atomic electrophilicity index of 103 elements of the periodic table, in terms of force concept. In the present report, we have applied electrophilicity equalization principle to compute molecular electrophilicity index and subsequently we have computed the dependent variable half-wave potential for quinone families, *viz.* benzoquinone, naphthoquinone and anthraquinone, through linear regression analysis, considering molecular electrophilicity as an independent variable. The ansatz suggested for the computation is:

$$E_{1/2} = -1.011 + 0.005\ \omega$$

The results illustrate a significant correlation of electrophilicity index with reduction potential of quinones family. We have also compared our computed half-wave potential values with those obtained experimentally for the test set data. A nice conformity was found between the predictions and the experimentally obtained half-wave potential values.

Keywords: Electrophilicity Index, Half-wave Potential, Quinones

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