ISCBC-2016

22nd ISCB International Conference

Abstract Book

22nd ISCB International Conference
6-8 February 2016
Uka Tarsadia University, Surat, India

Recent Trends in Affordable and Sustainable Drug Discovery and Developments

Organized by:
Indian Society of Chemists & Biologists
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ISCBC-2016

Recent Trends in Affordable and Sustainable Drug Discovery and Developments

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From the desk of
ISCB President & General Secretary

Prof. Anamik Shah

Dr. P.M.S. Chauhan

We are very happy to inform you that the **Indian Society of Chemists and biologists**, Lucknow, jointly organising its 22th international conference with **Uka Tarsadia University**, Bardoli, near **Surat** from **6th – 8th February, 2016 (Sat-Mon)**.

It is a matter of great pleasure that the focal theme of the 22st International Conference of ISCB is **'**Recent Trends in Affordable and Sustainable Drug Discovery and Developments'. 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, UK, Germany, France, Belgium, Sweden, Italy and many other will participate as keynote/invited speaker 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 400-700 young researchers & post doctoral researchers from entire country who will take part as oral/poster presentators.

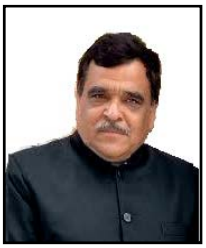
We are glad that the scientific committee is bringing out an abstracts book covering the presentations to be made during ISCBC-2016**.** Our sincere thanks are due to the members of organizing committee. During this conference a number of eminent scientists and technologists of the country and overseas 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 3Keynote lecture,8 plenary lectures,45 invited lectures by the eminent scientists from India and abroad.33 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. We are looking to the galaxy of speakers and young participants who made this conference a memorable event. We extend our warm welcome to all National and International delegates from pharmaceutical companies, research organization, universities and academic institutes wish them very happy stay at Bardoli, near Surat. Now Finally I take this opportunity to express my sincere thanks and gratitude to members and office bearers of organizing committee of 22st International Conference (ISCBC-2016).

(Prof. Anamik Shah)
President, ISCB

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

Message

Prof. (Dr). D. R. Shah



I am happy to note that Department of Chemistry, Uka Tarsadia University and ISCB – Lucknow are jointly organizing a first international conference on "Recent Trends in Affordable and Sustainable Drug Discovery and Developments". The conference aims to provide a knowledge base in the area of drug discovery and allied chemistry. It will bring together leading chemists, medicinal chemists, pharmacologists, biotechnologists, and other professionals from different parts of India and abroad to discuss and present the latest important developments in drug discovery and therapeutics.

It is also worth noting that this also gives an opportunity to young scholars to present their findings and learn from experiences of deliberations of esteemed scientist.

At this juncture I wish to congratulate the spirited efforts put in by the entire team of Department of Chemistry, Uka Tarsadia University for their whole hearted contributions to provide the best possible academic environment and make your stay comfortable.

I extend my best wishes to the organizing committee for successful organization and make this International Conference a grand success.

Prof. (Dr). Dinesh R. Shah
Provost
Uka Tarsadia University,
Maliba campus, Bardoli, Surat
E-mail: dinesh.shah@utu.ac.in

Message

Prof. K R. Desai

It indeed gives me a sense of pride in welcoming all the eminent scientists and young researchers in the International conference on **"Recent Trends in Affordable and Sustainable Drug Discovery and Developments"** to **UKA TARSADIA UNIVERSITY,** jointly organized by **Department of Chemistry, Uka Tarsadia University, Surat and Indian Society of Chemists and Biologists,** Lucknow during 6 – 7th February, 2016.

It is certain that the conference on Drug discovery and development is need of present scenario. Discovery of a new drug is a time consuming and very expensive business it has been estimated that it takes 8-10 years of sustained efforts of chemists, pharmacologists and physicians to bring a new product in market using modern drug discovery tools. It is also a very promising field for young researcher as it offers great employment opportunities.

This conference aim is to provide a platform for Chemists, Pharmacists, Botanists, Zoologists, Microbiologists, and many other along with Biotechnologists and Physicists to come together and make some academic deliberations, so that at the end a workable and useful recommendation can be made.

This is one of the happiest moments in the life of the Department of Chemistry as we are organizing a **First International conference.** Moreover Department of Chemistry has started many new programmes for her vertical growth. One of our targeted programs was to organize a international conference and today is the day when this dream has been realized.

I am thankful to all the member of the organizing committee for their hard work and support. Special thanks are due to all learned invited speakers who will deliver expert lectures of great relevance in Today's world. A very large number of delegates from various countries and different parts of India are participating in this conference. I am sure that each one of them will enjoyed the deliberation and as a Director, Department of Chemistry I wish to welcome each one of them and last but not list, I also wish to thank all the Guests, Professors, Scientist, Teachers, Students and representative from industry for coming to UKA TARSADIA UNIVERSITY to attend the conference. I hope that these days that we spend together will become a meaningful experience in itself.

Prof. Dr. K R. Desai
Director, Department of Chemistry
Uka Tarsadia University, Maliba campus, Bardoli, Surat
E-mail: kishor.desai@utu.ac.in

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February 6-8, 2016

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SCIENTIFIC PROGRAMME

Saturday, February 6, 2016

9.00 AM - 10.30 AM	**Registration**	
10.30 AM - 12.00 PM	**Inaugural Session**	
10:30AM	UTU Song	
10:35AM	Deep Pragatya and Ganesh Vandana and Flower welcome	
10:40AM	Welcome Address	**Prof. K. R. Desai**
10:50AM	Introduction to ISCB	**Dr. P.M.S. Chauhan, Gen. Secretary, ISCB**
11:00AM	Presidential Address	**Prof. Anamik Shah, President, ISCB**
11:10AM	Provost Address	**Dr. Dinesh R Shah**
11:15AM	ISCB Award Distribution	
11:30AM	Address by Chief Guest	**Naranjibhai Patel**
11:35AM	Address by Guest of Honour	**Dr. Amul Desai**
11:45AM	Keynote Lecture	**Prof. Sukh Dev Lala** New Delhi, India **Ayurvedic drugs repository: A cost effective modern drug search**
12:15PM	Vote of Thanks	**Organising Secretary**
12.15 PM - 12.30 PM	**High Tea**	

Session – I

Chairpersons: Prof. Michael D. Threadgill and Prof. Christophe LEN

PL-1 12.30 PM - 1.00 PM	**Jyoti Chattopadhyaya** Professor & Chair, Program of Chemical Biology, Dept. of Cell & Molecular Biology, Uppsala University, Sweden **Cross-talk amongst Neighbours in DNA and RNA and Self-assembly. An Unequivocal NMR evidence**
PL-2 1.00 PM - 1.30 PM	**Rui Moreira** iMed.ULisboa, Faculdade de Farmácia da Universidade de Lisboa, Av. Prof. Gama Pinto, Lisboa, Portugal *Abstract Awaited*
1.30 PM - 2.00 PM	**Lunch**

Parallel Session – II A

Chairpersons: Prof. H. Ila and Prof. Kishor Jain

IL-1 2.00 PM - 2.20 PM	**Branko Stanovnik** University of Ljubljana, Aškerčeva, Ljubljana, Slovenia **METAL-FREESYNTHESIS OF FUNCTIONALIZED HETEROCYCLES ENAMINONESIN THE SYNTHESIS OF HETEROCYCLIC SYSTEMS. [2+2] CYCLOADDITIONS, RING EXPANSION REACTIONS AND OTHER TRANSFORMATIONS**
IL-2 2.20 PM -2.40 PM	**Balasubramanian Gopalan** Chief Scientific Officer & Executive Director, Drug Discovery Research, Orchid Pharma Ltd, Chennai, India **Synthetic challenges in Drug Discovery Chemistry Research in Indian Pharma Industry**
IL-3 2.40 PM - 3.00 PM	**P. M. S. Chauhan** Professor (AcSIR), Senior Principal Scientist, Medicinal and process Chemistry Division,CDRI, Lucknow **Current Challenges in Drug Discovery: Design and Synthesis of Nitrogen Heterocycles as Novel therapeutic Agents**
4.00 PM - 4.20 PM	**Tea**

Parallel Session – II B

Chairpersons: Prof. Branko Stanovnik and Prof. Rui Moreira

IL-4 2.00 PM - 2.20 PM	**Carmen Nájera** Departamento de Química Orgánica and Centro de Innovación en Química Avanzada (ORFEO-CINQA), Universidad de Alicante, Apdo. 99, E-03080 Alicante, Spain **Asymmetric Synthesis of Highly Substituted Biological Active Prolines by 1,3-Dipolar Cycloadditions of Azomethine Ylides**

IL-5 2.20 PM - 2.40 PM	**Shubhankar Kumar Bose** Institut für Anorganische Chemie, Julius-Maximilians-Universität, Am Hubland, 97074 Würzburg, Germany **Zinc-Catalyzed Borylation of Alkyl and Aryl Halides with Alkoxy Diboron Reagents: An Efficient Synthetic Route to Alkyl and Aryl Boronates**
IL-6 2.40 PM - 3.00 PM	**Diwan S Rawat** Coordinator, M. Tech (Chemical Synthesis and Process Technologies), Department of Chemistry, OSD, University Press and Head Graphic Art Centre, Provost, Jubilee Hall, University of Delhi, Delhi-110007, India **Covalent hybridization: An innovative approach of drug discovery**
4.00 PM - 4.20 PM	**Tea**

Parallel Session – III A

Chairpersons: Prof. K. R. Desai and Dr. V. K. Tandon

PL-3 3.00 PM - 3.20 PM	**Anil Kumar Singh** Professor, Department of Chemistry, IIT Bombay, Powai, Mumbai **Organic Nanoparticles - drug design, diagnosis and delivery systems**
IL-7 3.20 PM - 3.40 PM	**H. Ila** New Chemistry Unit, Jawahar Lal Nehru Centre for Advanced Scientific Research, Bangalore-560064, India **Organic Synthesis Towards Greener Pastures**
IL-8 3.40 PM -4.00 PM	**Miguel Yus** Departmento de Química Orgánica and Centro de Innovación en Química Avanzada (ORFEO-CINQA), Universidad de Alicante, 03080 Alicante, Spain **Discovering new applications of chiral *N*-sulfinyl imines in asymmetric synthesis**
IL-9 4.00 PM - 4.20 PM	**Veela B. Mehta** Consultant, Columbus, Ohio, USA Neurodegeneration in the Multiple sclerosis brain: Role of iron
4.20 PM - 4.40 PM	**Tea**
IL-10 4.40 PM - 5.00 PM	**Virinder S Parmar** Bioorganic Laboratory, Department of Chemistry, University of Delhi, New Delhi, India **Biocatalytic Synthesis of Polymeric Nanoparticles useful in Theranostic and Drug Delivery Applications**
IL-11 5.00 PM - 5.20 PM	**Ashok K Prasad** Professor, Department of Chemistry, University of Delhi, Delhi- 110 007 **Glucose-based Macromolecular and Polymeric Architecture of Importance**

Parallel Session – III B

Chairpersons: Prof. Anil Kumar Singh and Prof. Ashok K Prasad

IL-12 3.00 PM - 3.20 PM	**Wafaa M. Abdou** Professor of Applied Organic Chemistry, Division of Chemical Industries, National Research Centre, Dokki, Cairo, Egypt **N, S-Bisphosphonic acids in prevention of inflammation and bone loss associated with adjuvant arthritis**
IL-13 3.20 PM - 3.40 PM	**Christophe LEN** Université de Technologie de Compiègne Centre de Recherches de Royallieu, F-60205 Compiègne, cedex, France **Green chemical synthesis and processing in water**
IL-14 3.40 PM - 4.00 PM	**Ashoke Sharon** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India-835215 HSP modeling, design & synthesis of new molecules as possible antivirals
IL-15 4.00 PM - 4.20 PM	**Rajneesh Misra** Department of Chemistry, Indian Institute of Technology Indore, Indore, M.P., India **Mechanochromism in benzothiadiazole derivatives**
4.20 PM - 4.40 PM	**Tea**
IL-16 4.40 PM - 5.00 PM	**Farukh Arjmand** Department Of Chemistry, Aligarh Muslim University, Aligarh U.P. 202002, India **De novo tailored design of new metal-based drugs or drug precursors for antitumor chemotherapy: Structure elucidation by Single X-ray crystallography and their in vitro binding and cytotoxicity profile**
IL-17 5.00 PM - 5.20 PM	**Sandeep Chaudhary** Department of Chemistry and Materials Research Centre, Malaviya National Institute of Technology Jaipur, Jawaharlal Nehru Marg, Jaipur-302017, India **Perspective and Challenges in Antimalarial Chemotherapy: Design and Synthesis of Novel Artemisinin Analogues as Antimalarials**

Poster Session –I

Chairpersons:

5.20 PM – 7.00 PM	**Poster Numbers 1-80**
7.00 PM – 8.30 PM	**Cultural Programme**
8.30 PM	**Dinner**

Sunday, February 7, 2016

Parallel Session – IV A

Chairpersons: Dr. Vijay Kumar Challa and Prof. Virinder S Parmar

PL-4	**Anamik Shah** Department of Chemistry, Saurashtra University, Rajkot, India

9.00 AM - 9.30 AM	**Collaborative Drug Research in India: The Current Contexts and Future Directions**
PL-5 9.30 AM - 10.00 AM	**Michael D. Threadgill** Professor of Medicinal Chemistry, Department of Pharmacy & Pharmacology, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom **Adventures in naphthalene chemistry – synthetic approaches to potent cyclopropa¬benz¬indole (CBI) cytotoxins**
IL-18 10.00 AM - 10.20 AM	**Mukesh Kumar Madhra** Chemical Research Division, Sun Pharmaceutical industries Limited, Gurgaon, Haryana, 122001, India **Challenges in Implementing Quality By Design: Practical Approaches for Process R&D and Manufacturing**
IL -19 10.20 AM - 10.40 AM	**Ramendra Pratap** Department of Chemistry, University of Delhi, North campus, New Delhi-110007, India **Chemistry of substituted acetonitriles**
IL -20 10.40 AM - 11.00 AM	**Vishnu K Tandon** Professor, Department of Applied Chemistry, Institute of Engineering and Technology, Lucknow-226020, India **Regioselective synthesis of polycyclic heterocycles that potently induce apoptosis in cancer cells**
IL -21 11.00 AM -11.20 AM	**Athina Athanasios Geronikaki** School of Pharmacy, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece **Synthesis and in silico biological activity evaluation of new N-substituted pyrazolo-oxazin-2-one systems**
11.20 AM - 11.40 PM	Tea

Parallel Session – IV B

Chairpersons: Prof. Athina Geronikaki and Dr. P. M. S. Chauhan

IL-22 9.00 AM - 9.20 AM	**Rachna Sadana** Assistant Professor of Biology and Biochemistry, Department of Natural Sciences, University of Houston-Downtown, One Main Street, Houston, TX-77002 **Integrating Research into Curriculum as High Impact Educational Practice Enriches Actinobacteriophage Database in Addition to Improving Student Learning**
IL-23 9.20 AM - 9.40 AM	**Rakesh Shukla** Chief Scientist & Head, Division of Pharmacology, CSIR-Central Drug Research Institute, Lucknow, India **Hypertension a risk factor for memory impairment: ACE inhibitors a useful therapy**
IL-24 9.40 AM - 10.00 AM	**N C Desai** Department of Chemistry, Mahatma Gandhi Campus,Bhavnagar University,

	Bhavnagar-364002, Gujrat, India **Contemporary Researchon nitrogen containing non-nucleoside reversetranscriptase inhibitors**
IL-25 10.00 AM - 10.20 AM	**Kishor S. Jain** Principal & Professor (Med.Chem.), Rasiklal M. Dhariwal Institute of Pharmaceutical Education and Research (RMDIPER), Chinchwad, Pune-411019, Maharashtra, India **Synthesis ,Docking study and Evaluation of novel antihyperlipidemic halogenated methylthieno[2,3-d]pyrimidines, with some molecular targets related to hyperlipidemia – an investigation into their mechanism of action**
IL -26 10.20 AM - 10.40 AM	**Brijesh Kumar** Sophisticated Analytical Instrument Facility Division, CSIR-Central Drug Research Institute, Lucknow-226031, India **Evidence based research for quality control of Indian Medicinal Plants using HRMS and LC-MS/MS instruments**
IL -27 10.40 AM - 11.00 AM	**Kamala K .Vasu** Assistant Director, Dean of Student's Affairs & Head, Department of Medicinal Chemistry, B.V.Patel PERD Centre, S.G.Highway, Thaltej,Ahmedabad-380 054, Gujarat, India **Adenosine Receptors and Inflammation in Neurodegenerative Disorders**
IL -28 11.00 AM -11.20 AM	**Anil Kumar Dwivedi** Division of Pharmaceutics, Central Drug Research Institute, Lucknow-226031, India **Analytical studies on standardized extract of a new chemotype of *Withania somnifera* Dunal (NMITLI 118RT+)**
11.20 AM - 11.40 PM	Tea

Parallel Session-V A

Chairpersons: Prof. Christophe LEN and Dr. Kamlakar Avasthi

IL-29 11.40 AM - 12.00 PM	**Vinay Tripathi** S&T Management Unit, CSIR-CDRI, Lucknow, India **Intellectual Property Rights; An Overview**
IL-30 12.00 PM - 12.20 PM	**Jawahar Lal** Senior Principal Scientist & Head, Pharmacokinetics & Metabolism Division, CSIR-Central Drug Research Institute, Lucknow 226 031, India **PopulationPharmacokineticmodelingin optimizing drug development**
IL-31 12.20 PM - 12.40 PM	**Sanjeev K. Shukla** Senior Scientist (CSIR-CDRI)/Asst Professor (AcSIR), NMR Lab., Sophisticated Analytical Instrument Facility, CSIR-Central Drug Research Institute, Lucknow 226 031, India **NMR-based Metabolomics to study the tissue specificity, seasonal and geographical variations in *Alstonia scholaris***
IL-32	**Bapu B. Shingate**

12.40 PM - 1.00PM	Assistant Professor, Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431 004, India **Stereoselective Syntheses of Naturally Occurring 20-epi Cholanic Acid Derivatives and Other Bioactive Compounds From 16-Dehydropregnenolone Acetate**
1.20 PM - 2.20 PM	**Lunch**

Parallel Session-V B

Chairpersons: Dr. Bapu B. Shingate and Dr. Brijesh Kumar

IL-33 11.40 AM - 12.00 PM	**Okram Mukherjee Singh** Professor, Department of Chemistry, Manipur University, Canchipur, Imphal-795003, Manipur, India **Indole derivatives and indole based alkaloids from dithiocarboxylates**
IL-34 12.00 PM - 12.20 PM	**R. K. Singh** Head, Division of Toxicology, CSIR- Central Drug Research Institute, Lucknow, India **Invention of A New Male Antifertility Injection- RISUG in India for 21st Century**
IL-35 12.20 PM - 12.40 PM	**Rajeev Sakhuja** Assistant Professor, Department of Chemistry, BITS Pilani, Pilani Campus, Rajasthan 333031, India **Functionalized Heterocycles: Scope & Applications**
IL-36 12.40 PM - 1.00PM	**Ajay K. Sah** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan **Design, synthesis and application of N-glycoconjugates as multi targeting drugs**
IL-37 1.00 PM - 1.20 PM	**Kamlakar Avasthi** Central Drug Research Institute, Lucknow-226031, India **Conformational control due to Arene interactions in Flexible Pyrazolo[3,4-*d*]pyrimidine core Based Models**
1.20 PM - 2.20 PM	**Lunch**

Parallel Session-VI A

Chairpersons: Prof. Anshu Dandia and Dr. Rakesh Shukla

PL-6 2.20 PM - 2.50 PM	**Nigel G. J. Richards** School of Chemistry, Cardiff University, Park Place, Cardiff, CF10 3AT, United Kingdom **Inhibiting Asparagine Biosynthesis in Human Cells: A New Approach to Developing Anti-Cancer Agents**
IL-38	**Premysl Mladenka** Charles University in Prague, Faculty of Pharmacy in Hradec Králové, Department

2.50 PM - 3.10 PM	of Pharmacology and Toxicology, Czech Republic **Are flavonoids a possible source of new cardiovascular drugs?**
IL-39 3.10 PM - 3.30 PM	**Prakash C. Jha** Central University of Gujarat, Sector-30, Gandhinagar, Gujrat, India **Multiscale Approach to Drug designing and Challenges for Next Millennium**
IL-40 3.30 PM -3.50 PM	**Indresh Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani-campus 333 031, Rajasthan, India **Aminocatalyzed Transformations of Dicarbonyls: Asymmetric Synthesis of Medium Sized Nitrogen Heterocycles**
O-1 3.50 PM - 4.00 PM	**Chandralata Bal** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi-835215, India **Amino acid ester analogs as cardiac CASQ2 depolymerization inhibitor**
O-2 4.00 PM - 4.10 PM	**Naval P. Kapuriya** Department of Chemistry, Shree M. & N. Virani Science College, Saurashtra University, Rajkot 360 005, Gujarat, India **DEVELOPMENT OF VITAMIN E-DERIVATIVES AS AKT INHIBITORS & ANTICANCER AGENTS**
O-3 4.10 PM -4.20 PM	**Pratibha Yadav** Center for Rural Development & Technology, IIT Delhi, Haus Khas, New Delhi, India **Synthesis of sulfoxide from sulfide using Plant Peroxidase**
4.20 PM - 4.40 PM	**Tea**

Parallel Session-VI B

Chairpersons: Dr. Jawahar Lal and Vinay Tripathi

PL-7 2.20 PM - 2.50 PM	**Rakhi Chaturvedi** Professor, Department of Biosciences and Bioengineering (BSBE), Associate Dean, Alumni Affairs and External Relations, Indian Institute of Technology-Guwahati, Guwahati- 781039, Assam, India **Screening and isolation of natural products from plant tissue cultures for the development of a new lead drug agent from the genus *Spilanthes***
IL-41 2.50 PM - 3.10 PM	**Devdutt Chaturvedi** Department of Applied Chemistry, Amity School of Applied Sciences, Amity University Uttar Pradesh (AUUP), Lucknow Campus, Lucknow-226028, U. P., India **Greener and efficient approaches for the syntheses of biologically potent scaffolds**
O-4 3.10 PM - 3.20 PM	**Ritu Kapoorr** Green Synthesis Lab, Department of Chemistry, University of Allahabad, Allahabad 211002, India **Visible Light Catalyzed Photooxidative Heterocyclization of Semicarbazones**

	for the Synthesis of 1,3,4-Oxadiazoles
O-5 3.20 PM - 3.30 PM	**D.N.Singh** Department of Chemistry, K.S.Saket PG College, Dr.RML Avadh University, Faizabad-224001, India **Plant Derived Lead Molecules as Pharmacologically Active Agents**
O-6 3.30 PM - 3.40 PM	**Vivek K. Vyas** Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad 382481, Gujarat, India **DESIGN OF 2-SUBSTITUTED BENZIMIDAZOLE DERIVATIVES AS PROCASPASE-3 ACTIVATORS AND APOPTOSIS INDUCER: 3D QSAR, DOCKING AND IN SILICO ADMET STUDY**
O-7 3.40 PM - 3.50 PM	**Hardik Bhatt** Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad 382 481. India **Design, Synthesis and Anti-HIV Activity of Novel Quinoxaline Derivatives**
O-8 3.50 PM - 4.00 PM	**Sanjeev Kumar** Molecular Biology and Genetics Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560064, India **Unexpected functional implication of a stable succinimide: a novel mechanism for structural stability in *Methanocaldococcus jannaschii glutaminase* (MjGATase)**
O-9 4.00 PM - 4.10 PM	**Rahul Shrivastava** Department of Chemistry, Manipal University, Jaipur-302007, Rajasthan, India **A novel, facile, rapid protocol for the one pot green synthesis of imidazoheterocyclicscaffolds viathree component condensation reactions**
O-10 4.10 PM - 4.20PM	**Anil Kumar** Synthetic Organic Chemistry Lab Shri Mata Vaishno Devi University, Katra, J&K, India **Chiral Cobalt(III) Complexes: Hydrogen Bond Donor Catalysts for Enantioselective Organic Synthesis**
4.20 PM - 4.40 PM	**Tea**

Parallel Session-VII A

Chairpersons: Dr. A. K. Dwivedi and Prof. Diwan Singh

IL-42 4.40 PM - 5.00 PM	**Dalip Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani 333 031, Rajasthan, India **Organoiodine reagents in the construction bioactive heterocycles**
O-11 5.00 PM - 5.10 PM	**Thokchom Prasanta Singh** Chemistry Department, Manipur University, Canchipur-795003, Manipur, India **Convenient synthesis of Green/Cyan Fluorescent Proteins Chromophoreusing Amino acids**

O-12 5.10 PM - 5.20 PM	**Nasimul Hoda** Department of Chemistry, Jamia Millia Islamia, New Delhi- 110025, India ***De-Novolead* optimization of potent Plasmodium falciparum phosphoethanolamine methyltransferase inhibitors**
O-13 5.20 PM - 5.30 PM	**Mousumi Kar** College of Pharmacy, IPS Academy, Indore, Madhya Pradesh, India **Development and in vitro-in vivo evaluation of hollow gastro retentive microspheres of an anti-diabetic drug prepared by emulsification solvent evaporation method**
O-14 5.30 PM - 5.40 PM	**Navin B. Patel** Department of Chemistry, Veer Narmad South Gujarat University, Surat-395 007, India **4-[2-(5-Ethylpyridin-2-yl)ethoxy]benzaldehyde and its analogs: A useful pharmacophore for antibacterial, antifungal and antitubercular agent**
O-15 5.40 PM - 5.50 PM	**Jibon Kotoky/ R. Elancheran** Drug Discovery Laboratory, Life Sciences Division, Institute of Advanced Study in Science and Technology, Guwahati-781035, India **Design & Development of therapy for Prostate Cancer based on Synthetic & Semi synthetic molecules**
O-16 5.50 PM - 6.00 PM	**Girish Chandra** Department of Chemistry, Central University of Bihar, Gaya, Bihar, India **Synthesis of Fluoro Analogue of Neplanocine A: Their Antiviral and Antitumor Activities**
O-17 6.00 PM - 6.10 PM	**Ranjan C. Khunt** Chemical Research Laboratory, Department of Chemistry, Saurashtra University, Rajkot-360005, Gujarat, India **Attribution of Disparate Dimedone Derivatives: Synthesis as well Docking Studies against 5-HT_{2A} Receptor**
O-18 6.10 PM - 6.20 PM	**Mohsin Y. Lone** CCG@cug Lab, School of Chemical Sciences, Central University of Gujarat, Gandhinagar 382030, Gujarat, India **Molecular Modeling Perspective of the Inhibitors Binding to Vinca Domain of Tubulin**
O-19 6.20 PM - 6.30 PM	**Mohd Athar** CCG@cug Lab, School of Chemical Sciences, Central University of Gujarat, Gandhinagar 382030, Gujarat, India **Appraisinglead-likeness descriptors for commercially available organic compounds**
O-20 6.30 PM - 6.40 PM	**Pravin Dudhagara** Department of Biosciences, Veer Narmad South Gujarat University, Surat-395007, India **Enzymes Mediated Synthesis and Characterization of Potent Antimicrobial Gold Nanoparticles against MDR bacteria and Development of Antimicrobial Surgical Suture**

Parallel Session-VII B

Chairpersons: Prof. R. K. Singh and Prof. Rakhi Chaturvedi

IL-43 4.40 PM - 5.00 PM	**Parthasarathi Das** Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu-180001, India **C/N-Arylation Chemistry: Development of Synthetic Tools for Medicinal Chemist**
O-21 5.00 PM - 5.10PM	**Vartika Srivastava** Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati, Assam, India **Screening of two important alkaloids from cell suspension cultures of *Tinospora cordifolia* (Willd.) Miers ex Hook. F. & Thoms using high-throughput screening methods**
O-22 5.10 PM - 5.20 PM	**Raja Gopal Reddy M** Lipid Biochemistry Division, National Institute of Nutrition, Jamai Osmania, Hyderabad-500 007, Telangana, India **Stearoyl CoA desaturase 1 (SCD1): A key target to control the development of non-alcoholic fatty liver disease (NAFLD) - study from an experimental model**
O-23 5.20 PM - 5.30 PM	**JignasaSavjani** Institute of Pharmacy, Nirma University, S.G. Highway, Ahmedabad, India **Design and Synthesis of Mefenamic acid Derivatives as Anti-inflammatory Agents**
O-24 5.30 PM - 5.40 PM	**Hitendra M. Patel** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **An efficient synthesis of some novel mannich products bearing quinoline nucleus and their microbial studies**
O-25 5.40 PM - 5.50 PM	**Gajjar Krishna** Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad - 382481.Gujarat, India **Exploratory& *in-silico* Studies, Design and Synthesis of GPR40 Modulators**
O-26 5.50 PM - 6.00 PM	**Kalpana Chauhan** School of Chemistry, Shoolini University, Solan, Himachal Pradesh, India **Microwave Synthesis and Bio-evaluation of CystineBased Bio-conjugates of Benzothiazole analogs**
O-27 6.00 PM - 6.10 PM	**JalpaTrivedi** Department of Science &Humanities, Indus University, Ahmedabad, Gujarat, India **An effective method for the synthesis of tetra substituted Pyrazine containing nucleoside analogues**
O-28 6.10 PM - 6.20 PM	**Gitu Pandey** Pharmaceutics Division, CSIR- Central Drug Research Institute, Jankipuram Extension, Lucknow-226031, India **Frankincense oil based nanoemulsified carrier system for synergistic effect**

	and improved delivery of docetaxel
O-29 6.20 PM - 6.30 PM	**Manoj Kumar Choudhary** Discipline of Inorganic Materials and Catalysis, Central Salt and Marine Chemicals Research Institute (CSIR-CSMCRI), Bhavnagar- 364 001, Gujarat, India **Enantioselective Henry reaction of trifluoromethyl ketones and aldehydes using chiral copper(II)-complex and their applications**
O-30 6.30 PM - 6.40 PM	**P S Desai** Department of Chemistry, Arts, Science and Commerce College Kholwad, Kamrej Char Rrasta, Surat 394 185, India **Inhibitory action of piperazine derivatives on mild steel corrosion in hydrochloric acid solutions**

Poster Session –II

Chairpersons: Dr. K. Avashthi and Dr. Jawahar Lal

6.40 PM – 7.30 PM	**Poster Numbers 81 onwards**
7.30 PM – 8.30 PM	**Cultural Programme**
8.30 PM	**Dinner**

Monday, February 8, 2016

8.00 AM – 9.00 AM	**Spritual Lecture by Swamiji at Sankri Swami Narayana Temple**

Session –VIII

Chairpersons: Prof. Jyoti Chattopadhyaya

Keynote -2 9.30 AM - 10.00 AM	**M M Sharma** Mumbai, India **Chemistry & Allied subjects: Current status & future directions**
PL-8 10.00 AM - 10.30 AM	**Orazio Antonio Attanasi** Department of Biomolecular Sciences, Section of Organic Chemistry and Organic Natutal Compounds, University of Urbino "Carlo Bo", Via I Maggetti 24, 61029 Urbino, Italy **Cultivating over thirty years the passion to build heterocycles from 1,2-diaza-1,3-dienes: the force of imagination**
IL-44 10.30 AM -10.50 AM	**Sivapriya Kirubakaran** Assistant Professor, Bioengineering & Chemistry, IIT-Gandhinagar, Gujarat, India **Targeting DNA Damage/ Repair pathways: Towards Novel therapeutics for cancer**
IL-45 10.50 AM -11.10 AM	**Jyoti Singh** ACS International India Pvt Ltd (earlier Sci-Edge Information) 501-3, Jeevan

	Heights, Thorat Colony, Erandwane, Pune–411004, India **Locating evasive patents of process/technologies & importance of indexed databases**
O-31 11.10 AM -11.20 AM	**Rajesh Kakadiya** Center of Excellence, National Facility for Drug Discovery Complex, Department of Chemistry (UGC SAP & DST –FIST sponsored), Saurashtra University, Rajkot – 360 005, Gujarat, India **QUINOLINE DERIVATIVES AS ANTICANCER AGENT**
O-32 11.20 AM -11.30 AM	**Shah Raj Ali** Department of Chemistry, D.S.B. Campus, Kumaun University, Nainital 263 002, India **Zinc hexacyanidocobaltate(III) nanoparticles catalyzed oxidation of benzyl alcohol**
O-33 11.30 AM -11.40 AM	**Vidhi Shah** Shah-Schulman Center for Surface Science and Nanotechnology, Dharmsinh Desai University, Nadiad-387001, Gujarat, India **Dynamics of Pluronics and their application as novel vesicular nanocarrier for drug solubilisation**
IL-46 11.40 AM -12.00	**Songhui Wang** China *Abstract Awaited*
Keynote-3 12.00 -12.30 PM	**Rashmi Barbhaiya** Co-Founder & CEO and Managing Director at Advinus Therapeutics Pvt Ltd, India **R&D Models for Addressing Affordability and Accessibility of Medicines**
ISCB Award Lectures 12.30 PM – 1:00 PM	**ISCB Award for Excellence** **Govindsamy Mugesh** Professor, IISc, Banglore, India
	ISCB Young Scientist Award **Arun Kumar Shukla** Assistant Professor, IIT Kanpur, India
1.00 PM - 1.40 PM	**Valedictory Session**
1.40 PM - 2.30 PM	**Lunch**
2:30 PM – 4:30 PM	**ISCB General Body**

KEYNOTE

Keynote-1

Ayurvedic drugs repository: A cost effective modern drug search

Sukhdev Lala

New Delhi, India

Sukh Dev received the MSc (1945) from Panjab University, Lahore (now in Pakistan), PhD (1950) from Indian Institute of Science (IISc), Bangalore, and DSc (1960) also from IISc. He was conferred DSc (*hc*) by Bundhelkhand University, Jhansi (2000) and also by IIT Delhi (2008). He served as Research Associate (1948-53) and Lecturer (1953-1959) at IISc; Research Associate (1957) at University of Illinois, Head, of the Division of Organic Chemistry, National Chemical Laboratory, Pune (1960-74), and Research Director, Malti-Chem Research Centre, Vadodara (1974-88). He was Visiting Professor, Stevens Institute of Technology (1968), University of Georgia (1969), and University of Oklahoma (1970-71). Currently, he is Visiting Professor at the Dr BR Ambedkar Centre for Biomedical Research, University of Delhi, and is also consultant with several chemical companies.

Academic & Research Achievements: Sukh Dev made significant contributions to our knowledge of organic chemistry by uncovering scores of novel, complex, plant secondary metabolites such as zerumbone, himachalenes, malabaricol, cheilanthatriol, kodocytochalasins, bakuchiol, guggulsterones, guggultetrols; development of new techniques and processes: silver nitrate-silica gel (for thin layer chromatography, organic reactions in a solid matrix, heterolytic cleavage of homoallylic alcohols), and concepts: Absolute Stereochemistry Biogenetic Rule. He worked on the Indian economic raw materials, such as lac, Indian turpentine oil, *devadaaru*, and Indian medicinal plants. Longifolene, a typical component of Indian turpentine was converted into useful aroma compounds, which are being manufactured not only in India, but also in foreign countries. Carene, another characteristic constituent of this oil, was fashioned into several commercially important molecules. Himachalenes, hydrocarbons from *devadaaru*, were recognised as effective against ectoparasites and have been commercialised as a veterinary drug. Several Ayurvedic crude drugs were investigated and evaluated for their therapeutic claims. For example, *guggulu* is claimed in Ayurveda for treating lipid disorders. Investigations led to the isolation of compounds (guggulsterones) responsible for this activity, and products based on this are being manufactured not only in India, but also by several parties abroad. Currently, there is much scientific interest in these molecules globally. Bakuchiol, a compound isolated from baakuchi, has been converted into a highly potent juvenoid, and has been successfully evaluated for its use in sericulture. He has more than 390 scientific publications to his credit including 55 patents. Ninety two students received their PhD under his direct supervision. He is the author of 10 books, and has contributed chapters in over 18 other books.

Other Contributions: Sukh Dev served on the Editorial Advisory Board of *Tetrahedron* and *Tetrahedron Letters* (1976-95), *Tetrahedron Asymmetry* (1990-95) and *Dictionary of Organic Compounds*, 5th Edn.

Awards and Honours: Dr Sukh Dev was conferred the Sudborough Medal by IISc (1949), Guha Research Medal by IISc (1958), SS Bhatnagar Award (1964), Acharya PC Ray Medal by Indian Chemical Society (1970), Dr KG Naik Gold Medal by MS University, Baroda 1977), Vishwakarma Medal by INSA (1979), Ernest Guenther Award by American Chemical Society (1980), Distinguished Alumni Award by IISc (1980), VASVIK Award (1980), FICCI Award (1980), Professor TR Seshadri 70th Birthday Commemoration Medal by INSA (1981), Meghnad Saha Medal by INSA (1987), Satyendra Nath Bose Research Professorship by INSA (1988-93), TWAS Award in Chemistry (1988), Srinivasan Ramanujan Birth Centenary Award by Indian Science Congress

Association (1992), Lifetime Achievement in Chemical Research and Education Award by Indian Chemical Society (1999), Lifetime Achievement in Chemistry Award by Chemical Research Society of India (2000), and Padma Bhushan (2008). He was elected Fellow of the Indian Academy of Sciences, Allahabad (1974), the Academy of Sciences for the Developing World (1992); President, Indian Chemical Society (1978-79), Organic Chemistry Division, IUPAC (also Co-opted Member, Titular Member, Secretary, 1983-85, and Vice-President); and Trustee (1983-) and Chairman (1987-91), National Organic Symposium Trust, India.

Keynote-2

Chemistry & Allied subjects: Current status & future directions

Man Mohan Sharma

Mumbai, India
E-mail: mmsharma@bom3.vsnl.net.in

Man Mohan Sharma obtained Bachelor of Chemical Engineering (1958) from Bombay University and subsequently MSc (Tech) in 1960. He obtained PhD (Chemical Engineering) (1964) at Cambridge University with PV Danckwerts. In 1964, he returned to India as Professor at the University of Bombay, and later became Director of the University Department of Chemical Technology (UDCT), now ICT (Institute of Chemical Technology - A Deemed University). He remained Director, UICT for 33 years. He has been honored by several universities including IITs by honorary doctorates.

Academic & Research Achievements: Sharma made monumental contributions to chemical engineering science and technology. His studies on Bronsted based catalysis in CO2 hydration (published in the *Transactions of Faraday Society*) and subsequently kinetics of COS absorption in aqueous amines and alkanolamines brought out linear free energy relationship between CO2 and COS absorption in solutions of amines and alkanolamines. He has contributed extensively on the role of microphases in multiple reactions which he pioneered. He also became an independent Editor of *Chemical Engineering Science* at a young age. He taught different subjects in chemical engineering and encouraged his doctoral students, from the very beginning, to publish independently their work in renowned journals. He mentored 71 PhDs and was an active consultant to industry.

Other Contributions: Under his stewardship, UICT got autonomy of UGC. He brought about all-around improvement in all the departments of the Institute leading to exceptionally high number of PhDs each year based on the number of faculty members. He served in Petroleum and Natural Gas as Chairman of the SAC and in the SAC to Cabinet and PM. He was INSA Council Member (1980-82) and Vice President (1987-88).

Awards and Honours: Professor Sharma is a recipient of a number of prestigious academic honours and awards including the SS Bhatnagar Prize in Engineering Sciences, Moulton Medal of the Institution of Chemical Engineers, and UK Leverhulme Medal of the Royal Society. He was awarded the Padma Vibhushan (2001), and Padma Bhushan (1987) by the President of India. He was INSA President (1989-90). He is a Fellow of the Indian Academy of Sciences, Bangalore, Honorary Fellow of the National Academy of Sciences (India), Allahabad, Fellow of the Royal Society, London. Subsequently he was elected Honorary Fellow by the Royal Academy of Engineering and is Foreign Associate of the US National Academy of Engineering.

Keynote-3

R&D Models for Addressing Affordability and Accessibility of Medicines

Rashmi Barbhaiya

Co-Founder & CEO and Managing Director at Advinus Therapeutics Pvt Ltd., India
E-mail: rashmi.barbhaiya@gmail.com

Rashmi H. Barbhaiya, Ph.D. is a Pharmaceutical Executive with over 30 years of experience in Pharmaceutical R&D. Leveraging his two decades of large pharma experience and to address key issues affecting pharma R&D productivity and return on investment (ROI), he has developed novel R&D models involving polycentric and globally networked innovation and for de-risking drug discovery. He has a unique blend of management experience in Drug Discovery, Development and Life Cycle Management. He is one of the founders of Advinus Therapeutics, a research-based Tata Enterprise pharma company located in Bangalore and Pune, India. He was also CEO and Managing Director of the Company from 2005 to 2015.

Dr. Barbhaiya started his industrial pharmaceutical career in 1980 with Bristol-Myers Company in United States where he spent the next 21 years. The diversity of his background and experience has played a key role in speedy and successful discovery & development of a number of drugs for the treatment of a variety of diseases such as, AIDS and other infectious diseases, cancer, depression, anxiety, hypertension, CHF, diabetes and mild to moderate pain, including migraine.

In the year 2002, he returned to India to join Ranbaxy as the President of R & D and led a team of over 900 professionals involved in drug delivery and innovation-driven new drug research and development activities as well as R&D for developing generic drugs. He is credited for attracting world-class experienced scientists from overseas and for enhancing an innovation-driven culture to create one of the leading pharmaceutical R & D organizations in India. He was instrumental in creating an R & D alliance between Ranbaxy and GSK, the first of its kind for an Indian company. The alliance between Medicine for Malaria Venture (MMV) and Ranbaxy has introduced a cost-effective life-saving drug for the treatment of malaria. This is an example of addressing affordability and accessibility of medicines – the treatment cost for this proprietary life-saving drug in India is $2.

In the year 2005, he co-founded Advinus Therapeutics Pvt Ltd; a Tata enterprise. This was his first entrepreneurial venture. Advinus has a unique business model involving value-creating drug discovery and growth-driven service organization focusing on pre- and early-clinical development. Advinus is created to address fundamental issues of R& D productivity, speed, efficiency and cost. Under his leadership, Advinus has established an impressive record of novel R &D alliances with large pharma that includes path-breaking alliance with Takeda. This innovation driven company was founded with equity of about $20 M.

He obtained Ph.D. degree in Clinical Pharmacology from the St. Bartholomew's Hospital Medical College, University of London. He continued his education through post-doctoral training at the University of Florida and University of Wisconsin. His scientific contributions have resulted in over 150 publications. He has served on the Editorial Boards of Antimicrobial Agents and Chemotherapy as well as Biopharmaceutics and Drug Disposition journals. Dr. Barbhaiya has received a number of awards for his scientific contributions. Some of these include AAPS Fellow, AAPS Meritorious Manuscript Award, AAiPS Outstanding Achievement Award, Ranbaxy Award for Excellence in Pharmaceutical Research, India Life Sciences Person of the Year 2007 by Burrill& Company and BioSpectrum Entrepreneur of the Year 2010.

PLENARY

PL-1

Cross-talk amongst Neighbours in DNA and RNA and Self-assembly. An Unequivocal NMR evidence

Jyoti Chattopadhyaya

Department of Cell & Molecular Biology, University of Uppsala, Box 581, S-75123 Uppsala, Sweden
Email: jyoti@boc.uu.se

1. The basic building blocks of Nucleic acids, RNA and DNA, are (a) Nucleobase, (b) Pentofuranosyl-sugar and (c) the Phosphate dioester. Althouigh they are interalia covalently linked, yet each one of them are self-aware of their individual Chemical statusquo, which means that they can read each others pH-dependent chemical integrity. This has been evidenced by high-field NMR in my lab.
2. Although Nobel prize was given to Watson and Crick for the structure DNA duplex, it was up till now thought that the Single-strand DNA and RNA are random coil. Recently, we have given NMR evidences showing that indeed single-strand, depending upon its sequence compositiion, are stacked or destacked and self-organized when stacked, with a definite helicity.
3. What it is to have a sequence context in DNA or RNA? We have shown that each nucleobase with a specific specific sequence of DNA or RNA do "talk" and "cross-talk" to each other electrostatically and modulate each others Chemical properties, such as pKa. This in turn serves as a recognition signal with a certain energy penalty in pH dependent manner.

References:

Some key references see also my list of publications and PDFs in www.boc.uu.se:

1. Free download of my Review "Stereoelectronic Effects in Nucleosides and Nucleotides and their structural implications" by J. Chattopadhyaya et al, Uppsala University Press, ISBN 91-506-1351-0, Distributor: Bioorganic Chemistry, Uppsala University, 1999.
2. J. Chattopadhyaya et. J. AM. CHEM. SOC. 2003,125 , 9948-9961; J. Org. Chem. 2003, 68, 1529-1538; J. AM. CHEM. SOC. 2004,126 , 2862-2869.
3. Very grateful to all of my 287 corkers, so far, for all these and other studies doccumented in my publication list at www.boc.uu.se

PL-2

Rui Moreira

iMed.ULisboa, Faculdade de Farmácia da Universidade de Lisboa, Av. Prof. Gama Pinto, 1649-003 Lisboa, Portugal
Email: rmoreira@ff.ul.pt

Abstract Awaited

PL-3

Organic Nanoparticles - drug design, diagnosis and delivery systems

Anil Kumar Singh

Department of Chemistry, Indian Institute of Technology Bombay, Mumbai – 400 076, India
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Nanoscience and technology is poised to play significant role in nanomedicine, particularly with regard to improved drug design, diagnosis, and drug delivery. However, many challenges must be overcome if the application of nanoscience and technology is to fully realize the anticipated benefits and improved therapies. In the context of nanomedicine, some of the challenges include nanoparticle's size uniformity, biocompatibility, specific drug targeting and delivery, biological behaviour and reducing toxicity while maintaining therapeutic effects. Engineered nanoparticles are an important tool to overcome some the challenges. In this respect, design and synthesis of nanoparticles of small organic molecules is attracting a great deal of attention. The electronic properties of organic nanoparticles (ONPs) differ fundamentally from those of inorganic nanoparticles because of weak intermolecular forces of attraction. Further, the ONPs allow much increased variability and flexibility in synthesis of materials and investigation of their physicochemical properties. Much attention is also being paid towards design of ONPs with enhanced fluorescence capability as fluorescent organic nanoparticles (FONs) are considered to be of great significance in disease diagnosis.

Despite numerous important advances, the synthesis and formulation of small organic molecules-based nano-structured materials with good control of particle shape and size in aqueous media still remains a major challenge. Research efforts have focused on developing special formulation techniques to disperse the solid organic materials into water, maintain the dispersion for a certain time period, and functionalize the ONPs. In this scenario, we have focused our attention on understanding the factors that control the size and size distribution of nanoparticles, and also the fluorescent emission efficiency. Towards these goals we have synthesized ONPs of cholesteryl compounds by microemulsion method and studied the effect of increasing hydrophobicity on the size of the nanoparticles. We have also designed 3-styrylindole-based ONPs capable of enhanced fluorescence emission. It has been found that nanoparticles of strong donor-acceptor styrylindoles, synthesized by re-precipitation method, can have J-type morphology with reduced face-to-face intermolecular interaction, and such ONPs show highly enhanced fluorescent emission. These ONPs were spherical with mean diameter of about 20-30 nm. In addition to these studies, we have also explored the possibility of using caging concept for controlled delivery of drugs and bioactive compounds, and to this goal we have designed several chromophores, which are light-activatable under biologically benign conditions.

This talk, while giving an overview of the recent accomplishments in the field of nanoparticles of small organic molecules as applied in drug design, delivery, and discovery of improved therapeutics and diagnostics will focus on our efforts towards the design and synthesis of nanoparticles of i) cholesteryl esters with the objective of understanding the factors that control nanoparticle formation and size, and ii) styrylindoles and other related light emitting molecules with the objective of understanding the effect of aggregation on the fluorescence efficiency of the nanoparticles, and iii) aspects of light-induced release of bioactive compounds from molecular cages as promising tool for controlled-drug delivery. Further, the challenges and opportunities in the design of ONPs with possible therapeutic scenarios and future inroads in other fields will also be highlighted.

PL-4

Collaborative Drug Research in India: The Current Contexts and Future Directions

Anamik K. Shah*

Centre of Excellence in Drug Discovery NFDD Complex, Department of Chemistry, Saurashtra University, Rajkot -360005(India)
Vice-Chancellor, Gujarat Vidyapith, Ashram Road, Ahmedabad – 380014(India)
E-mail: anamik_shah@hotmail.com; anamik_shah@gujaratvidyapith.org

Abstract Awaited

PL-5

Adventures in naphthalene chemistry – synthetic approaches to potent cyclopropabenz-indole (CBI) cytotoxins

Michael D. Threadgill,* Elvis A. Twum, Michael C. B. Kenny, Andrew S. Thompson, Timothy J. Woodman

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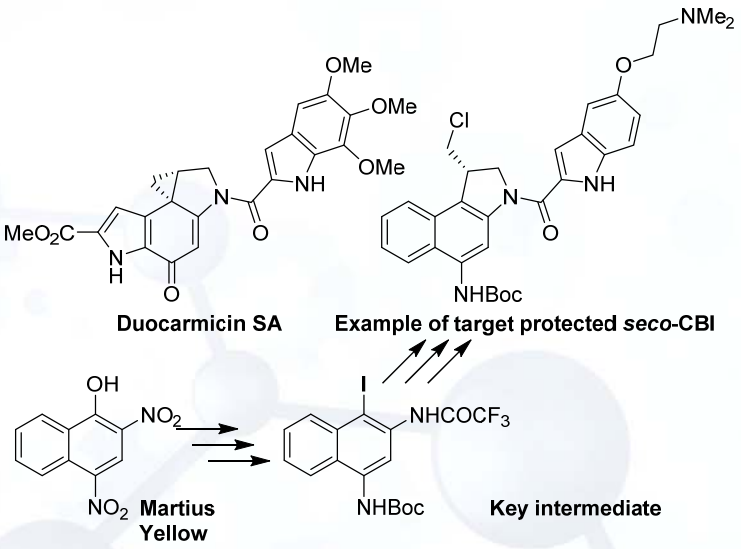
Chemotherapy of prostate cancer is limited by systemic toxicity. An attractive new approach is to deliver a potent cytotoxin selectively to the tumour in the prostate by a prodrug. Our research is developing such a prodrug by attaching a potent cytotoxin to a water-soluble carrier polymer through a link that is cleaved by prostate-specific antigen (PSA), an extracellular protease which is widely distributed but is catalytically active only in the prostate. To reduce the drug loading on the carrier polymer, a super-potent cytotoxin is required. Duocarmycin SA is a cyclopropapyrroloindole (CPI) which is cytotoxic at low pM concentrations. Both bind in the minor groove of DNA, placing the strained spirocyclopropane close to a nucleophilic site.



We are synthesising derivatives of functionalised protected *seco*-CBIs. Release will trigger Winstein cyclisation to the active CBI cytotoxin.Martius Yellow carries the correct substitution pattern on the naphthalene to access the Key Intermediate but there were major challenges protecting the nitrogens orthogonally. Martius Yellow was triflated and converted to 1-iodo-2,4-dinitronaphthalene but regio-selective reduction was not possible. Reduction gave naphthalene-1,3-diamine. Regioselective trifluoro-acetylation, Boc protection and iodination gave the Key Inter-mediate. Selective removal of one Boc group from 1-iodo-2,4-bis(BocHN)naphthalene was investigated, giving onlydeiodination. A cationic Wheland intermediate was observed by NMR. [1] Selective allylation at the 2-H and radical ring-closure with TEMPO set up the benzodihydroindole core of the target, with the two amines and the exocyclic OH fully orthogonally protected. Elaboration led to the target and analogues. [2]

The naphthalene chemistry developed in these routes and the biological activity of the CBIs will be discussed.

We thank Prostate Cancer UK.

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PL-6

Inhibiting Asparagine Biosynthesis in Human Cells: A New Approach to Developing Anti-Cancer Agents

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There is increased interest in how the alteration of key metabolic processes can enhance tumorigenesis, and in how these changes might be disrupted in anti-cancer therapies. There is ample evidence that asparagine depletion exerts a tumoricidal effect and the enzyme that mediates asparagine biosynthesis, asparagine synthetase (ASNS), has become of increasing interest as a drug target [1]. For example, knockdown of ASNS expression by small-interfering RNAs in androgen-response and castration-resistant prostate cancer lines inhibited their growth in media devoid of asparagine [2]. Similar effects of ASNS knockdown were observed in breast cancer cell lines [3]. Compounds that can be used to inhibit ASNS therefore represent potential anti-cancer drugs. In recent years, our group has identified the first potent inhibitors of human ASNS using structure-based methods for drug discovery [4,5] and has also constructed a working model (based on the crystal structure of *Escherichia coli* AS-B) [6] of how the inhibitor is bound within the enzyme. Progress in delineating the structural features that mediate inhibitor recognition and binding will be discussed in this lecture, together with the results of *in silico* screening calculations using an optimized model of ASNS complexed to a key reaction intermediate (unpublished observations). These docking studies have identified a new structural motif for ASNS inhibitors that should permit the development of compounds with improved cell permeability.

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PL-7

Screening and isolation of natural products from plant tissue cultures for the development of a new lead drug agent from the genus *Spilanthes*

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N-alkylamides are large and promising group of bioactive molecules classified as secondary metabolites which is majorly present in the genus *Spilanthes*. The herbal extracts of different plant species belongs to the genus *Spilanthes* is mostly used as a folklore remedies. The wide arrays of pharmaceutical activities are due to the presence of spilanthol and other important alkylamides. Therefore, to obtain the complete utilization of natural plant metabolites, a surge-on biotechnological tool, plant cell culture technology can be employed to produce the juvenile *in vitro* cultures for the extraction and analysis of metabolites. The systemic effect of metabolite followed by the regulatory product classification can be achieved evidently after screening phytochemicals. The evaluation of metabolite production from plant species noticeably and undoubtedly can afford the formulation of a lead drug which develops a great solution against the growing problem of multi-drug resistance parasites causing infectious diseases.

Keywords: Plant tissue culture; Plant extracts; *Spilanthes* sps; Spilanthol

PL-8

Cultivating over thirty years the passion to build heterocycles from 1,2-diaza-1,3-dienes: the force of imagination

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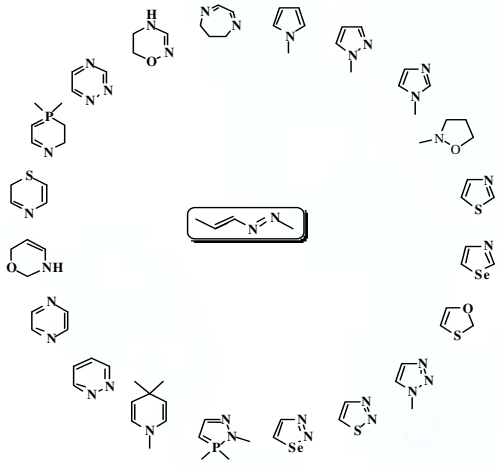
Pyrroles, pyrrolines, pyrazoles, pyrazolines, imidazoles, imidazolines, imidazolidindiones (hydantoins), 2-thioxoimidazolinones (2-thiohydantoins), isoxazolidines, thiazoles, thiazolines, thiazolidines, 2-iminothiazolidinones, selenazoles, selenazolines, 1,3-oxathioles, 1,2,3-triazoles, 1,2,3-thiadiazoles, 1, 2,3-selenodiazoles, 1,2,3-diazaphospholes, pyridines, pyridazines, dihydropyridazines, tetrahydropyridazines, pyrazines, dihydropyrazines, tetrahydropyrazines, piperazines, 1,3-oxazines, 1,4-thiazines, dihydro-1,4-thiazines, tetrahydro-1,4-thiazines, dihydro-1-aza-4-phosphinine, 1,2,4-triazines, tetrahydro-1,2,4-triazines, 1,2,4-oxadiazines, tetrahydro-1,4-diazepinones, 1,4-benzodiazepines and mixed heterocyclic systems have been obtained from 1,2-diaza-1,3-dienes.[1-19]



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INVITED

IL-1

METAL-FREESYNTHESIS OF FUNCTIONALIZED HETEROCYCLES

ENAMINONESIN THE SYNTHESIS OF HETEROCYCLIC SYSTEMS

[2+2] CYCLOADDITIONS, RING EXPANSION REACTIONS AND OTHER TRANSFORMATIONS

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Enaminones and relatedcompounds turned out to be extremelyversatilereagents in thesynthesis of manyheterocyclicsystems [1], includingmanynitrogencontainingnaturalproducts and their analogues [2].

Recently, wereportedregiospecificmicrowave-assisted [2+2], [4+2]cycloadditions and Michael additions of substituted 2-amino-3-(dimethylamino)propenoates and other enaminones, derived mostly from methyl ketones, with electron poor acetylenes, such as acetylenecarboxylates, and azodicarboxylates, whichgavehighlyfunctionalized 1-amino-4-(dimethylamino)buta-1,3-dienes as intermediatesforthepreparation of polysubstituted pyrroles, azapentalenes, triazafulvalenes, 2-heteroarylpyridines and their*N*-oxides, 1-aryl (orheteroaryl)imidazol-2-ones and otherheterocyclicsystems [3].

[2+2]Cycloadditions of substitutedacetyleneiminiumsalts toenaminones, ring-expansion reactions, rearrangements of heterocyclic systems and othertransformationswill be presented [4].

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IL-2

Synthetic challenges in Drug Discovery Chemistry Research in Indian Pharma Industry

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Pharma industry has the fundamentals that are going to lead to increased demand for health care where innovation is going to be critical for the next decade. With the ageing population & chronic illnesses increasing, there is going to be a great demand, even in emerging markets that will require innovation to deliver on those needs. Hence, commitment to R&D in Innovation-driven activities such as Drug Discovery, development of Chiral pharmaceuticals & Green chemistry, generating Intellectual Property are very critical for the future.

In order to make high potency drug molecules, one of the strategies (hybrid approach in Natural products) would be to combine two bioactive molecules belonging to a particular therapeutic category. In Drug Discovery Chemistry research, in the process of Lead generation, no factor is larger than the compounds for biological screens. In the syntheses of structurally diverse small molecules, Synthetic Organic Chemists face several challenges in developing new strategies for target molecules with efficiency in time & greenness. In addition, Diversity Oriented Synthesis in Lead-generation poses a greater challenge.

Many of the problems faced in the syntheses of different target molecules in varied projects would be discussed in detail.

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IL-3

Current Challenges in Drug Discovery: Design and Synthesis *of Nitrogen Heterocycles as Novel therapeutic Agents*

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Drug research one of the important area of science. It is also very time taking and require multidisciplinary efforts.

Nitrogen heterocycles are constituted a major class of existing drugs. These compounds are widely distributed in nature and are essential to life process. They also play a vital role in the controlling the metabolism of all living cells. The activity of these molecules is attributed to their ability to interfere against several imortant biological target sites.

Keeping in view importance of nitrogen hetrocycles in antiparasitic area, we have synthesized novel heterocycles as antiparasitic agents . These heterocycles were synthesized by classical solution phase as well as on solid support. Several synthesized compounds have shown promising *in vitro* and *in vivo* antiparasitic activity against Malaria and Leshimania parasites. The design, synthesis and antiparasitic activity of these *novel therapeutic agents* will be discussed [1-6]

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IL-4

Asymmetric Synthesis of Highly Substituted Biological Active Prolines by 1,3-Dipolar Cycloadditions of Azomethine Ylides

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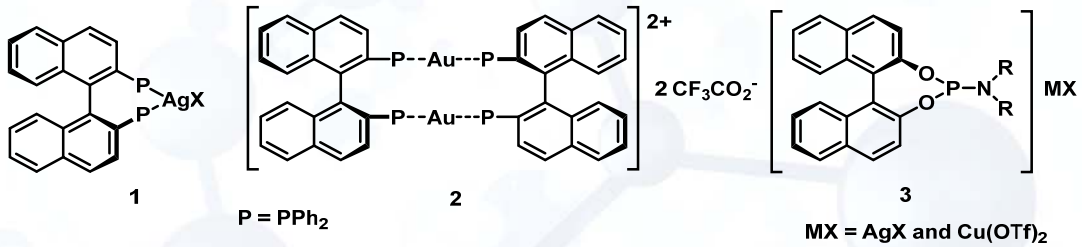
Metal-catalyzed 1,3-dipolar cycloadditions (1,3-DC) of azomethine ylides and dipolarophiles allowed the simultaneous formation of two carbon-carbon to give the corresponding pyrrolidines. The use of different chiral catalysts derived from binap and phosphoramidites as privileged ligands and silver, gold(I) and copper(II) salts for the enantioselective synthesis of highly substituted prolines by 1,3-DC of azomethine ylides with dipolarophiles is presented. The 1,3-DC using bidentate binap complexes gave good enantioselectivities for azomethine ylides when silver salts monomeric complexes **1**[1] and dimeric gold **2** trifluoroacetates [2] are used yielding *endo*-cycloadducts. In the case of monodentate ligands such as phosphoramidites, metal complexes **3** derived from silver salts have been used for the general 1,3-DC of different imino esters and dipolarophiles to afford *endo*-cycloadducts [3]. In the case of using nitroalkenes as dipolarophiles copper(II) triflate and also silver benzoate and triflate complexes **3** were the most appropriate catalysts affording *exo*-cycloadducts [4]. In addition, computational studies have also been carried out in order to explain the high enantioselection exhibited by these chiral complexes. This methodology has been applied to the synthesis of hepatitis C virus inhibitors blocking the viral RNA-dependent RNA-polymerase [5] and for the preparation of *exo*-4-nitroprolines, which are excellent chiral organocatalysts [6] and are precursors of farnesyltransferase inhibitors[7].



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IL-5

Zinc-Catalyzed Borylation of Alkyl and Aryl Halides with Alkoxy Diboron Reagents: An Efficient Synthetic Route to Alkyl and Aryl Boronates

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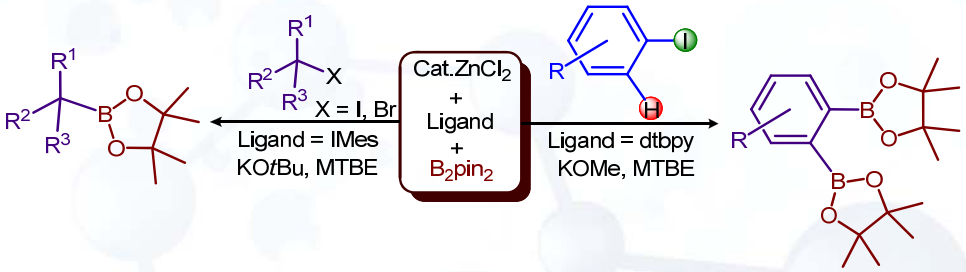
Organoboronates are important in medicinal chemistry in and of themselves, as well as being often used as synthetic intermediates for transition-metal catalyzed cross-coupling, conjugate addition and many other reactions [1, 2]. Considerable effort has been committed to their preparation using precious metals (such as Pd, Rh, Ir, etc.) and more recently, using non-precious metals (Cu, Ni, Fe). We have developed a new non-precious metal catalytic system based on a Zn(II)-NHC complex for the cross-coupling reaction of alkyl halides with diboron reagents, which represents a novel use of a group XII catalyst for the borylation reaction [3]. This approach achieves borylations of unactivated primary, secondary and even some tertiary alkyl halides to furnish alkylboronates, with good functional-group compatibility, under mild conditions. A related $ZnBr_2$-NHC catalyst system also borylates aryl halides [4] and, most recently, we have shown that $ZnCl_2$, in the presence of 4,4'-di-tert-butyl-bipyridine as the ligand, borylates both aryl C-X bonds and the C-H bonds adjacent to them [5]. The key results will be described.



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IL-6

Covalent hybridization: An innovative approach of drug discovery

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The design of new molecules with improved ADME properties along with effective pharmacological potency; lack of toxicity and devoid of resistance for the treatment of infectious diseases has remained a big challenge for the scientific community. In order to address these issues concept of hybrid molecules was put forward which deals with the covalent hybridization of two or more distinct pharmacophores into a single molecule that may lead to a hybrid molecule with improved efficacy [1-3]. This approach may solve the problem of drug resistance and reduce the undesired side effects [4]. The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials. Towards these goals we have synthesized various molecular hybrids and tested these for antimalarial, anti-Parkinson and anti-cancer activities and efforts will be made to present our recent work [5-20].

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IL-7

Organic Synthesis Towards Greener Pastures

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Present scenerio of organic synthesis in 21st century demands development of energy efficient processes from renewable starting materials with minimum waste production to reduce the environmental and health impact of chemical production.

'Small molecule heterocycles' play important role in both drug discovery and material science research providing one of the richest source of diversity, besides serving as rigid scaffolds for further display of a range of functionalities. Therefore design and development of new pathways leading to efficient synthesis of novel heterocycles, from easily accessible precurssors displaying skeletal and functional group diversity is emerging as an important area in both synthetic organic and medicinal chemistry.

Our recent efforts in this direction to develop new efficient synthetic methods for biologically important five and six membered heterocycles involving transition metal catalyzed cross coupling, C-H activation (atom economy reactions)(inter- and intramolecular C-heteroatom bond formation), domino and multicomponent reactions will be presented in the lecture.[1]

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1. Selected recent papers: (a) Review: H. Ila and H. Junjappa *Chimia* **2013,** *67*, 17. (b) A. Acharya, S. Vijay Kumar, H. Ila *Chemistry Eur. J.* **2015**, *21*, 17116. (b) A. Acharya, S. Vijay Kumar, B. Saraiah, H. Ila *J. Org. Chem.* **2015**, *80*, 2884.(c) A. Acharya, G. Parameshwarappa, B. Saraiah *J. Org. Chem.* **2015,** *80*, 414. (d) S. Vijay Kumar, B. Saraiah, G. Parameshwarappa, H. Ila *J. Org. Chem.* **2014**, *79*, 7961 (e) B. Raghava, G. Parameshwarappa, A. Acharya, H. Ila *Eur. J. Org. Chem.* **2014,** 1882. (f) S. Vijay Kumar, S. K. Yadav, B. Raghav, H. Ila *J. Org. Chem.* **2013**,*78*, 4960. (g) S. Yugandar, A. Acharya, H. Ila *J. Org. Chem.* **2013**,*78*, 3948. (h) S. Vijay Kumar, G. Parameshwarappa, H.Ila *J. Org. Chem.* **2013,** *78*, 7632. (i) S. Yugandar, N. C. Misra,, G. Parmeshwarappa, H. Ila *Org. Lett.* **2013**, *15*, 5250.

IL-8

Discovering new applications of chiral *N*-sulfinyl imines in asymmetric synthesis

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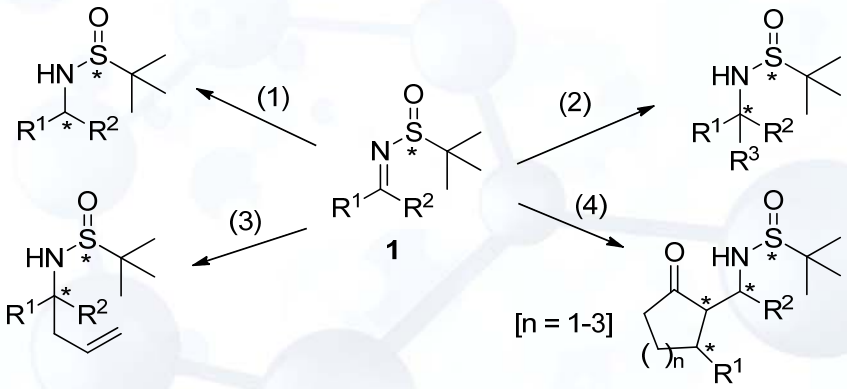
Chiral *N*-sulfinyl imines, especially the corresponding *N*-*tert*-butyl substituted derivatives **1** [1] are interesting starting materials in asymmetric synthesis because (a) they are easily accessible in both enantiomerically pure form, (b) the sulfinyl group activates the imine moiety towards nucleophilic substitution so, in the reaction with different nucleophiles an asymmetric induction takes place giving an diastereoenriched product, which can be easily separated into the corresponding pure diastereomers, and (c) the deprotection of the amino group, after the addition of the nucleophile can be easily achieved by simple treatment with hydrochloric acid. In this presentation, the reactivity and synthetic applications of these materials in the (1) ruthenium-catalyzed hydrogen transfer [2], (2) addition of alkyl zincates [3], (3) indium-promoted allylation [4] and (4) multicomponent reactions involving cycloalkenones and dialkyl-zinc reagents [5] will be considered. Especial attention is paid to the synthetic applications of the mentioned processes, mainly for the preparation of natural or unnatural alkaloids and amino acids [6].



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6. This work has been supported by the Spanish Ministerio de Ciencia e Innovación (MICINN) (Consolider INGENIO 2010 CSD2007-00006, CTQ2011-24151, and CTQ2011-24165), the Spanish Ministerio de Economia y Compe-titividad (MINECO) (projects CTQ2013-43446-P, CTQ2014-51912-REDC and CTQ2014-53695-P), FEDER, the GeneralitatValenciana (PROMETEO 2009/039 and PROMETEOII/2014/017), and by the University of Alicante.

IL-9

Neurodegeneration in the Multiple sclerosis brain: Role of iron

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Accumulation of iron in some white matter lesions of multiple sclerosis (MS) patients may contribute to the pathogenesis and progression of diseases. Our study explored the role of iron present in the white matter lesions. We performed (1) immunohistochemistry of human MS tissue and (2) in vitro iron uptake by M1-and M2-polorized human macrophages. Using iron staining of human autopsy tissue sections of MS patients, iron was detected primarily in non-phagocytosing macrophages at the edge of demyelinated lesions but not in myelin containing non-inflammatory M2 macrophages. Moreover, Iron containing tissue macrophages expressed proinflammatory M1 markers. Similarly, in cultured human macrophages (purified from healthy donor), exposed to iron, showed polarization-dependent iron uptake. Exposure of iron-laden macrophages to purified human myelin lead to depletion of iron from myelin-phagocytosing macrophages in all polarization states. Taken together our data shows that myelin downregulates intracellular iron retention in macrophages and thus perhaps myelin ingestion may regulate iron homeostasis via specific process(es).

IL-10

Biocatalytic Synthesis of Polymeric Nanoparticles useful in Theranostic and Drug Delivery Applications

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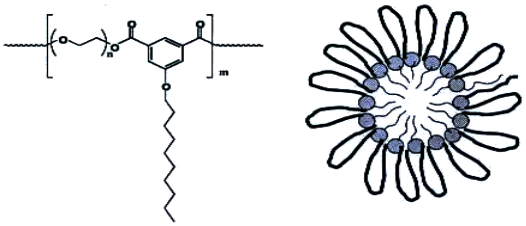
We have developed a chemo-enzymatic synthesis for novel amphiphilic polymeric nanoparticles based on PEG and PG having a broad range of additional chemical functionalities under mild conditions. Simplicity and versatility of this method for the synthesis of highly functionalized amphiphilic polymeric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

These unique alternating copolymer micellar **nanoparticles** have been used successfully for encapsulation of a large number of drugs of different classes and delivery vehicles targeted to human cancer cells expressing the underglycosylated mucin-1 antigen, which is found on almost all epithelial cell adenocarcinomas. The solubility of the chemotherapy drug doxorubicin increased by encapsulation in these **nanoparticles**, and cellular uptake, and hence cell death, was enhanced as compared to that with the free drug. The encapsulated taxol and doxorubicin showed significant enhanced activity against neuroblastoma cancer cells than anti-cancer drugs alone, and doxorubicin encapsulation showed 3-6 times better activity against pancreatic cancer cells.



Nanospheres with different linker molecules such as naturally occurring aspartic acid and glutamic acid have been prepared to assure non-toxic character of these materials and their biodegradability. The surface of these **nanospheres** is non-immunogenic as they are rich in PEG which does not interact with proteins. These polymers self assemble in water to produce **nanospheres** with a typical diameter of 10-70 nanometers. Critical micelle concentration for these micelles is low (0.25 millimolar).

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. The methodology developed for the synthesis of perfluorinated copolymers is highly flexible and efficient. The *in vitro* and *in vivo* studies on these **nanoprobes** are in progress. Recently we have synthesized cationic polymers that constitute of guanidine functional groups and poly(ethylene glycol) units. Because of their strongly basic character, guanidines are fully protonated under physiological conditions. The positive charge thus imposed on the molecule 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. These materials are non-toxic, 60 g material per kg body weight can be tolerated.

Based on lipase (*Candida antarctica* lipase B), oxidase (horse radish peroxidase) and their combination, the synthesis of pegylated polyelectrolytes have been developed. The pegylated macromers were polymerized and co-polymerized with various monomers of interest to generate a variety of tethered ion-conducting polymers for preparing quasi-solid electrolytes. The bio-derived non-crystallizable polymeric materials were used in formulating quasi-solid electrolyte compositions and incorporated into flexible dye-sensitized titanium oxide solar cells (DSSC). It was observed that the solar conversion efficiency of quasi –solid electrolytes incorporated solar cells depends strongly on the polymer microstructure used in formulating the redox electrolyte and our polymeric materials showed photovoltaic efficiency of upto 9.0 %.

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

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IL-11

Glucose-based Macromolecular and Polymeric Architecture of Importance

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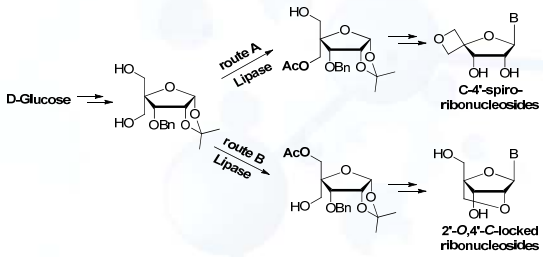
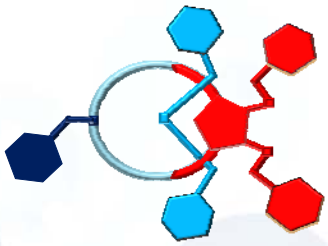
Nucleosides are among the most widely studied fundamental building blocks of biological system that are used as therapeutic agents to treat cancer, fungal, bacterial and viral infections. The ribose ring in the natural nucleosides experience rapid flipping between the two preferential conformations, *viz.* $C_{2'}$-*endo* (*S*-type) and $C_{3'}$-*endo* (*N*-type) due to the low energy barriers. The conformational behaviour of natural or modified nucleosides has demonstrated great importance in terms of their metabolic pathways and interactions with the biological targets. This has resulted in the synthesis of chemically modified nucleoside analogues having conformationally restricted pentofuranose ring. Prominent among these are the locked nucleic acid and spironucleosides.

The use of biocatalysts in the synthesis of nucleoside analogues 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 locked nucleic acid and C-4′-spironucleosides (Scheme 1). Further, we have used the modified sugar precursor for the synthesis of chiral crown ether analogs and [2]pseudorotaxanes.





[2]Pseudorotaxane

Scheme 1: Chemo-enzymatic Synthesis of *C*-4′-Spiro- & LNA Monomers

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IL-12

N, S-Bisphosphonic acids in prevention of inflammation and bone loss associated with adjuvant arthritis

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Bisphosphonates (BPs) are synthetic pyrophosphate mimics,which isnaturally occurring, where the chemically and enzymatically labile P-O-Pbridge has been replaced with a P-C-P bridge, making thesecompounds relatively resistant to chemical hydrolysis andcompletely resistant to enzymatic hydrolysis (Figure 1).BPs inhibit bone resorption by reducing osteoclast activity and inducing osteoclast apoptosis [Wafaa, et al 2015]. They are therefore, used for treatment post-menopausal osteoporosis in women and reducing the associated bone fracture risk.These BP-compounds bind strongly to calcium phosphate and inhibit its formation, aggregation and dissolution. Their affinity for the bone mineral represents the basis for their use in the treatment of many diseases associated with increased bone resorption. As described above, the BPs have been used for decades in the therapy of bone diseases but recently thesecompounds have been found to be active in many other fields, such as in the treatment of parasitic diseases cancers, and human rheumatoid arthritis[Wafaa, et al 2012]. We also utilized the high bone-joint-specificity of sulfur containing bisphosphonic acids with other chemical moieties of potential anticatabolic pharmacology for testing as novel class of compounds for the treatment of human rheumatoid arthritis[Wafaa, et al 2006]. The studied *S,N*-BP-acids were, therefore, designed to contain a latent (or free) thiol group that may bind to a metal atom in the active site of the matrix metalloproteinase (MMP). In this research work, we attempted to pavethe way to the study of the effects of these agents *S,N*-BP-acids on induction of apoptosis,and their first therapeutic application *in vitro* with myositisossificans (Figure 2).

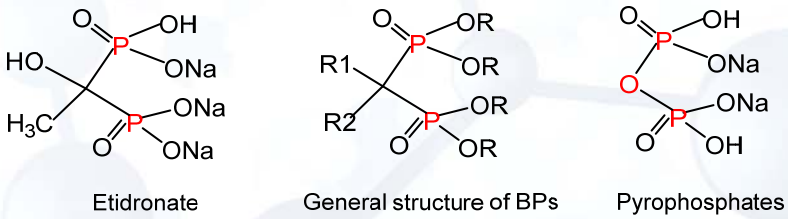

Figure 1

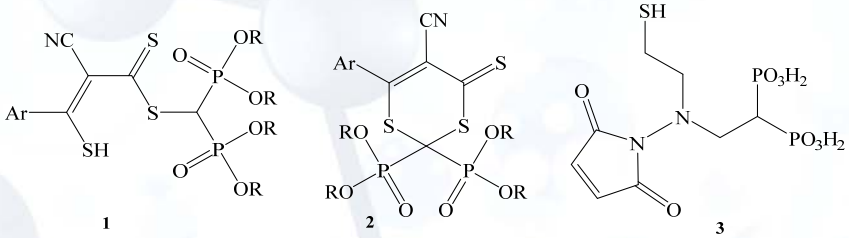

Figure 2. *S,N*-BP-acids: 1-3

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IL-13

Green chemical synthesis and processing in water

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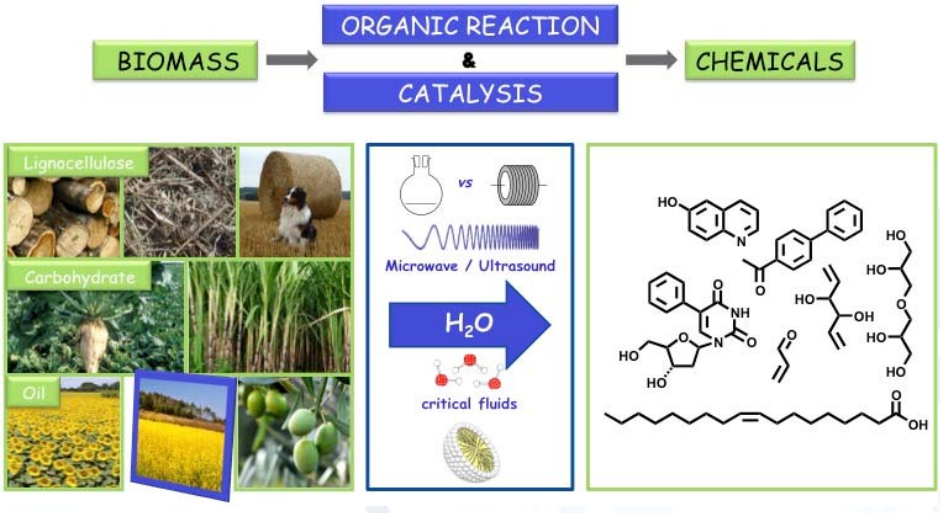
The design of environmentally friendly methodologies has been the driving force of scientists in recent years. In particular, the use of biomass-derived materials, green solvents and alternatives techniques has been investigated.

In thisconference, several green chemistryapproachesthattargetadvancedsynthesis and processeswillbepresented. Theseapproachesinclude: (i) green synthesis of quinoline and phenanthrolinederivatives in sole water usingmicrowave irradiation and hightemperature/pressure;[1] (ii) production of furfural fromD-xylose, xylane and hemicelluloseusingmicrowave irradiation and hightemperature/pressure;[2] (iii) conventionalmicellarcatalysis and magicphotochromicmicellarcatalysis[3] such as reductivepinacolcouplingaffording 1,2-diols *via* C-C bond creationbetweentwocarbonyl compounds; Pd-catalyzedTsuji-Trostreactionaffordingallylic analogues *via* C-C, C-N, C-S bond creations; Barton decarboxylationaffording new carboxylicacid or diacid*via* radical homologation.

Conception, synthesis and physico-chemicalpropertieswillbedetailed.



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IL-14

HSP modeling, design & synthesis of new molecules as possible antivirals

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The recent explorations on heat shock protein (Hsp) supports its emergence as a promising target to overcome drug resistance and latency in antiviral therapy. Modeling studies on Hsp suggest the binding of ATP in the N terminal region causes a conformational change that facilitates the N terminal interaction of the two monomers and a clamp like formation with a "lid" of amino acid residues enclosing the bound ATP. Thus the conformational changes in the ATP lid play an essential role in the activity of the protein. In ATP bound state, ATP lid exists in "closed" conformation and when the ATP is hydrolyzed or the protein is bound to an inhibitor, the ATP lid exists in "open" conformation. The modeling results suggest the newly synthesized compounds are able to modulate the Hsp in open conformation followed by its antiviral effect.Structure activity relationship (SAR) was analyzed with synthesized compounds on the basis of antiviral activities and cytotoxicity studies. Few compounds were found to be highly active with inhibitory potentials >90% at their highest non-toxic concentration of 1000nm. Structural rationale, modeling studies and biological activity suggest the possibility that this novel scaffold may be able to modulate Hsp, however detail biochemical mechanism are yet to be confirmed. *(Authors thanks to DBT (BT/PR14237/MED/29/196/2010), India for financial support.)*

IL-15

Mechanochromism in benzothiadiazole derivatives

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Conventional fluorescent dyes are poorly fluorescent in the solid state due to the phenomena called aggregation caused quenching (ACQ).[1] There are certain strategies by which the solid state emission can be enhanced. The Solid state emissive materials are of interest for variety of applications.[2] In this presentation, I will discuss about the strategies of enhancing the solid state emission and their mechanochromic behaviour.

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IL-16

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

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Cancer is a complex class of disease in which a group of cells divide uncontrollably beyond the normal limit, subsequently intruding to the near or distant tissues (metastasis), ultimately causing cell death. There are more than 100 phenotypes of cancers derived from numerous organs or tissues with multiple etiologies and endless combinations of genetic and epigenetic alterations. Therefore, **one**-drug-fits-**all** approach does not work for all the cancers. New rationale drug design strategies opt for tailored drug design involving the specific site of action at the target site possessing lower systemic toxicity which could arbitrarily be done by choosing appropriate metal ion and tailoring of ligand scaffold etc.

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

In continuation to our previous interest of designing new tailored drug candidates for antitumor chemotherapy, we have carried out synthesis of a few notably important metal-based drug entities 1) Chromone-appended Cu(II) drug entity $[C_{36}H_{50}CuN_8O_6]$ 2) ionic Sn(IV) iminodiacetic acid–piperazinediium conjugate $[C_8H_{17}N_3O_4Cl_4Sn]$ 3) $[C_{21}\ H_{22}\ Cu\ N_4\ O_7]$ 4) Ag(I) nalixidic acid-piperazine complex 5) Enantiomeric L/D- boc valine derived Co(II) and Fe(II) peptide conjugates $[C_{36}H_{56}CoN_4O_{10}]$ $[C_{36}H_{56}FeN_4O_{10}]$. Herein we will discuss their structure elucidation, *in vitro* DNA binding and cytotoxicity profile.

IL-17

Perspective and Challenges in Antimalarial Chemotherapy: Design and Synthesis of Novel Artemisinin Analogues as Antimalarials

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Malaria is still one of the major health problem in the whole world along with tuberculosis and AIDS. The parasite responsible for the vast majority of fatal malarial infections is *P. falciparum*. The first effective antimalarial drug was quinine, which was isolated from the bark of Cinchona. Since then malaria has been treated with quinoline-based drugs such as quinine, chloroquine, mefloquine and primaquine. Unfortunately, many *Plasmodium* strains have now become resistant to these drugs. Almost 42 years ago, the major breakthrough in malaria chemotherapy occurred when a new antimalarial structural prototype with a pharmacophoric peroxide bond in a unique 1, 2, 4-trioxane heterocycle i.e. artemisinin was isolated from *Artemisia annua* and brought great attention to the whole world in malaria chemotherapy. It met the dual challenges posed by drug-resistant parasites and rapid progression of malarial illness.

Available evidence proves that artemisinin and related peroxidic antimalarial drugs exert their parasiticidal activity subsequent to reductive activation by haem, released as a result of haemoglobin digestion by the malaria-causing parasite *Plasmodium*. This irreversible redox reaction produces carbon-centered free radicals, leading to alkylation of haem and proteins (enzymes), one of which-the sarcoplasmic endoplasmic reticulum ATPase PfATP6-may be critical to parasite survival.

The chemotherapy of malaria has benefited greatly from the semi-synthetic artemisinin derivatives such as dihydroartemisinin, artemether, arteether and artesunate as they rapidly reduce parasite burden, have good therapeutic indices and provide successful outcomes for the treatment of malaria. However, as a drug class, the artemisinins suffer from chemical (semisynthetic availability, purity and cost), biopharmaceutical (poor bioavailability and limiting pharmacokinetics) and treatment (non-compliance with long treatment regimens and recrudescence) issues that limit their therapeutic potential.

Our research programme had two major objectives: (a) to develop new antimalarials and especially effective against resistant malaria and (b) to develop efficient technologies for existing antimalarial drugs. As part of this programme and in search for better artemisinin analogues, we will discuss about our attempt that has been made to improve the antimalarial activity of artemisinin better than that of β-arteether. We will also discuss about the structure, conformation and stereochemistry of artemisinin skeleton by utilizing several synthetic strategies. Furthermore, synthesis and antimalarial testing of several new artemisinin analogues, exploring the antimalarial potency of artemisinin by carrying out structure-activity relationship, development of new biologically active scaffolds in artemisinin skeleton and the study towards the preparation of artemisinin- 1,2,4-trioxanes hybrid will be discussed.

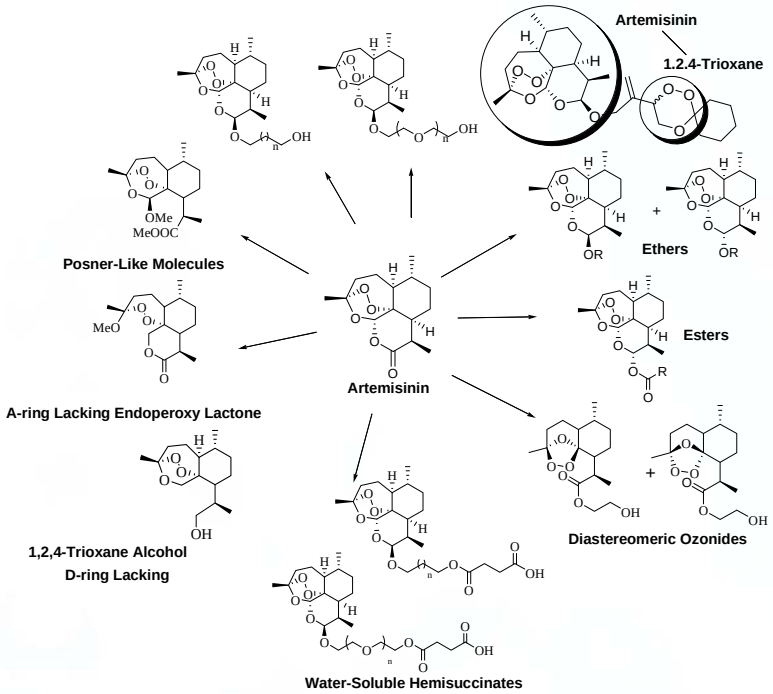

Figure 1: Structures of Artemisinin derivatives.

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IL-18

Challenges in Implementing Quality By Design: Practical Approaches for Process R&D and Manufacturing

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Developing a pharmaceutical quality system based on an integrated approach to risk management and science is today's need for a prospective risk-based approach to pharmaceutical product development **[1].**Attaining the "desired state" requires effective Quality by Design (QbD) implementation. It is a systematic approach to drug development that begins with predefined objectives and emphasizes product and process understanding and process control based on sound science and quality risk management**[2,3].**The focuses on practical approaches to accelerated QbD implementation by prioritizing process parameters for screening designs using statistical design of experiments (DoE), bridging the bench and the commercial design spaces using mixing and scale-up calculations,quantifyingprocess risk, Selecting suitable process analytical technology tools (PAT) etc are the key elements for arealistic implementation of QbD elements.

Since 2004, a number of working groups and pilot programs have sought to "incorporate elements of risk and quality by design throughout the life cycle of the product"**[4].**But even till 2014, implementation of QbD industrywide has been slow. So FDA has now "strongly suggested" QbD elements, and regulatory requirements are soon to be required in generic-drug applications. However, the pharmaceutical industry has yet to fully embrace QbD and will soon need to fundamentally change and/or evolve different modes of drug product development in-line with QbD concepts. The current challenges for QbD implementation are numerous. This talk serves as a QbD introduction and surveys the current state of QbD implementation. It focuses on an industry perspective with specific discussions regarding industry challenges.

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IL-19

Chemistry of substituted acetonitriles

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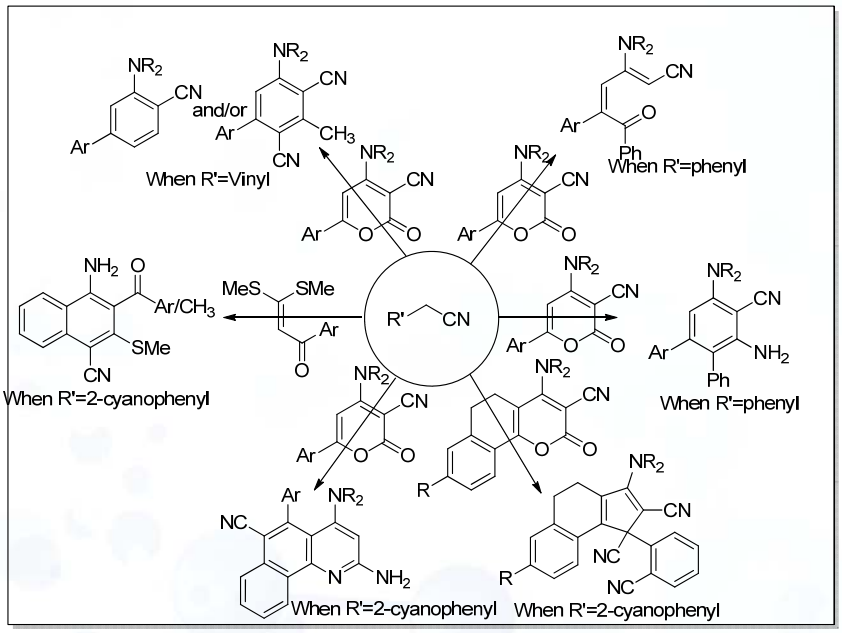

Various functionalized acetonitriles were used as precursor from several decades. Recently, we have picked up 2-cyanomethylbenzonitrile, benzyl cyanide and allyl cyanide and other acetonitriles and used them as a carbanion source to explore their chemistry. We have synthesized various functionalized naphthalenes in good to excellent yield using 2-cyanomethylbenzonitrile.[1,2] We have further explore 2-cyanomethylbenzonitrile as a carbanion source and isolated highly functionalized beno[*h*]quinolines on reaction with 2-pyranone.[3] Interestingly, use of 2-oxo-4-secamino-1-yl-5,6-dihydro-2*H*-benzo[*h*]chromene-3-carbonitriles in lieu of 2-pyranone provides 1-(2-cyano-phenyl)-3-*sec*.amino-1-yl-4,5-dihydro-1*H*-benz[*e*]indene-1,2-dicarbonitriles.[4] 1*H*-Naphtho[1,2-*d*]imidazole were also synthesized in three steps involving 2-(1-cyno-2,2-bis methylsulfanyl vinyl)-benzonitrile[1,5] as an intermediate obtained from 2-cyanomethylbenzonitrile. We have also used allyl cyanide to synthesized various functionalized biaryls. We have also used benzyl cyanide and synthesized various teraryls and enones under different reaction conditions.

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IL-20

Regioselective synthesis of polycyclic heterocycles that potently induce apoptosis in cancer cells

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Dibenzoxepine framework is commonly present as substructure in natural products of therapeutic significance. They are effective against H-29 human colon adenocarcinoma and MDA-MB-231 human breast cancer cells. We have devised an elegant regioselective synthesis of fused tetra and pentacyclic heteroarenes that potently induce apoptosis in cancer cells.

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IL-21

Synthesis and in silico biological activity evaluation of new N-substituted pyrazolo-oxazin-2-one systems

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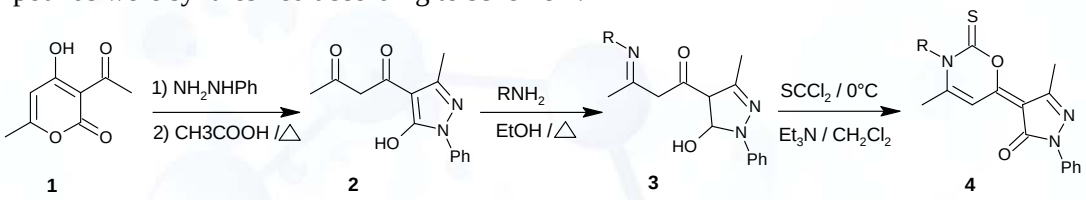
As members of the oxazinones' family are known to exhibit a variety of properties including anti-inflammatory and antimicrobial action, we designed and synthesised a new series of oxazinone derivatives hoping to result in novel multifunctional molecules. The in silico biological activity evaluation of the compounds and the in vitro evaluation of the cyclooxygenase inhibitory action of the compounds as a first estimation of their anti-inflammatory potential are presented in this paper.

Novel pharmacological actions can be found for N-substituted pyrazolo-oxazin-2-ones on the basis of computer-aided drug discovery approach with computer program prediction of activity spectra for substances (PASS).[1-4]

Compounds were synthesized according to scheme 1.



1 2 3 4

4a. R = $-CH_2CH_3$
4b. R = $-CH_2CH_2\ CH_3$
4e. R = C_6H_5-CH_2-
4f. R = $-C_6H_5$
4g. R = 4- $CH_3C_6H_4$
4h. R = 4 - $CH_3OC_6H_4$
4i. R = 4- BrC_6H_4
4j. R = 4 - ClC_6H_4

Replacement of the oxo group by isosteric thioxo group gave rise to an increase of the biological activity in many cases. [5-7]

Preliminary docking results for some of the compounds of the N-substituted pyrazolooxazin-2-one series and its thione analogues revealed that replacement of oxygen with the less electronegative sulfur could improve COX-1 inhibitory activity of the compounds.

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IL-22

Integrating Research into Curriculum as High Impact Educational Practice Enriches Actinobacteriophage Database in Addition to Improving Student Learning

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Undergraduate research has been recognized as an effective high impact practice in higher education. Engagement of undergraduate students in scientific research at early stages in their careers presents an opportunity to excite students about science, technology, engineering, and mathematics (STEM) disciplines and promote continued interests in these areas.Engaging large number of undergraduates in authentic scientific discovery is desirable but difficult to achieve.Science Education Alliance Phage Hunting Advancing Genomics and Evolutionary Science (SEA-PHAGES) is one of the top national program to engage students in discovery of new viruses, genome annotation, and comparative genomics.SEA-PHAGES is a two-semester, discovery-based undergraduate research course that begins with simple digging in the soil to find new viruses, but progresses through a variety of microbiology techniques and eventually to complex genome annotation and bioinformatics analyses. University of Houston-Downtown (UHD) has offered SEA-PHAGES course for past three years and have contributed by discovering 32 new bacteriophages. Eleven (35%) have been sequenced that belong to different (A, B, C, K and N) clusters, and 10 have been annotated. In addition to the strong impacts on bacteriophage research, the project has resulted in increased student persistence in STEM fields, and student self-identification with learning gains, motivation, attitude, and career aspirations.

IL-23

Hypertension a risk factor for memory impairment: ACE inhibitors a useful therapy

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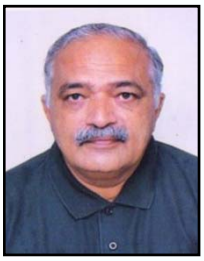
Clinical observations have indicated a positive correlation between cognitive decline and hypertension. We have demonstrated that hypertension renders the brain susceptible to memory impairment due to chronic neuroinflammation induced by repeated Lipopolysaccharide (LPS) administration (25 µg, ICV) on day 1, 4, 7 and 10 in spontaneously hypertensive rats (SHRs) but not in normotensive wistar rats (NWRs). We also showed that control SHRs exhibited exaggerated angiotensin converting enzyme (ACE) activity and expression, increased neuroinflammation, oxidative stress and β-secretases (BACE) expression without Aβ1-42 deposition in the brain. Chronic neuroinflammation induced by LPS further amplified the ROS generation and expression of BACE, Aβ1-42 deposition and memory impairment along with endothelial dysfunction, CBF reduction and increased RAGE expression and ERK1/2 activation in SHRs. In addition, we showed that perindopril (ACE inhibitor), at non-antihypertensive dose (0.1 mg/kg, p.o. x 15 days) prevented memory impairment by reducing oxidative stress, endothelial dysfunction, RAGE activation and amyloidogenesis in SHRs. This shows that central angiotensin system influences memory independent of the blood pressure modulating effect. Thus, we propose that ACE inhibitors might be useful as a therapeutic strategy to enhance neuroprotection particularly in reference to memory dysfunction in hypertensive subjects.

IL-24

Contemporary Researchon nitrogen containing non-nucleoside reversetranscriptase inhibitors



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The human immune deficiency virus-1 is the causative agent of the acquired immune deficiency syndrome (AIDS). So far, the only approved drugs for the therapy of HIV-1 infection are 3'-azidothymidine (AZT, Zidovudine) and recently 2',3'-didesoxyinosine (ddl, Didanosine), 2',3'-didesoxycytidine (ddC, Zalcitabine), stavudine (d4T) and lamivudine (3TC). Unfortunately, these drugs cause severe side effects such as thrombocytopenia,bone marrow toxicity and peripheral neuropathy.To avoid the sever toxicological disadvantages associated with the administration of nucleoside inhibitors and to contrast the rapid emergence of AZT resistant strains,recently a number of new type of non-nucleosides inhibitors of HIV-1 RT have been reported.Many researchers have attempted to identify non-nucleosides RT inhibitors usually via strategies involving broad screening of chemical inventories.As a consequence of these efforts,several non-nucleoside reverse transcriptase inhibitors(NNRTIs)of disparate structures have been discovered. Currently, nevirapine, delavirdine and efavirenz have been successfully used as drugs. Over and above, several protease inhibitors i.e. indinavir, nelfinavir etc. have been used as cocktail for the treatment of HIV patients.

In continuation to this, our group has started to synthesized and screened on anti-HIV activity of some nitrogen containing non-nucleoside reverse transcriptase inhibitorsasanti-HIV agents(i.e.quinazolines,4-oxo thiazolidines,2-imino-4-oxo thiazolidines and s-triazine derivatives.). In the present paper we have discussed the HIV virus life cycle, synthesis and mode of action of the drugs on HIV virus.

IL-25

Synthesis, Docking study and Evaluation of novel antihyperlipidemic halogenated methylthieno[2,3-*d*]pyrimidines, with some molecular targets related to hyperlipidemia – an investigation into their mechanism of action

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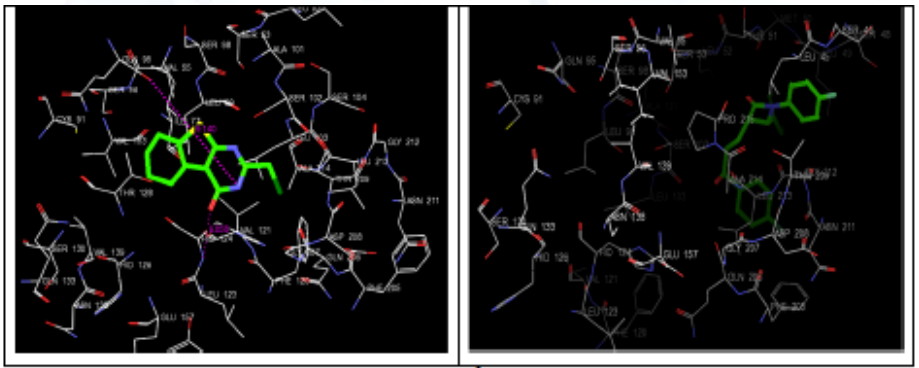
Identification and exploitation of novel molecular targets for discovery of new antihyperlipidemicdrugs is an important area of research. Twenty such drug targets are elaborated by the author, for their biochemical roles, structures, estimations, as well as, exploitation for new drug discoveryresearch. Few recently discovered drugs are based on such molecular targets shall be discussed.[1]. Further,An investigation [2,3] into the mechanism of the significantantihyperlipidemic action of some halogenated methylthieno[2,3-*d*]pyrimidines, synthesised under one-pot MWI methodology was carried out through docking experiments with six different molecular targets; Niemann Pick C1 Like1 protein (NPC1L1), ATP citrate lyase (ACL), C-reactive protein (CRP), lanosterol 14α-demethylase(LDM), squalene synthase (SqS) and farnesiod X-receptor (FXR) known to be implicated in the physiology of hyperlipidemia. The interactions of these were compared with the interactions of their respective co-crystallized native ligands at the active sites of these receptors. These comparisons are based on their docking parameters, as well as, types of interactions and vicinity with various amino acids in the active site pockets. The interactions of these synthesised compounds with the target, NPC1L1 were found to be the quite favourable as compared to those with the other targets assessed in this study.



a b

Keywords: Docking experiments; Antihyperlipidemic; halogenatedmethylthieno[2,3-d]pyrimidines; Molecular targets for hyperlipidemic research, MWI based synthesis

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IL-26

Evidence based research for quality control of Indian Medicinal Plants using HRMS and LC-MS/MS instruments

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Herbal medicines, also known as botanical medicines or phytomedicines, refer to the medicinal products of plant roots, leaves, barks, seeds, berries or flowers that can be used to promote health and treat diseases. Today, a vast range of drugs are either natural products or have been derived from them. Moreover increasing sales of herbal products indicate a worldwide concurrent surge of natural product use. Chemical fingerprinting has been demonstrated to be a powerful technique for the quality control of herbal medicines. A chemical fingerprint is a unique pattern that indicates the presence of multiple chemical markers within a sample. Similarly Natural products containing inherently large structural diversity are still a major source of bioactive agents. However many bioactive compounds have been re-discovered from new sources of natural products. To avoid it the identification of known leads at the early discovery step is highly desirable, a process known as dereplication provides an efficient tool for rapid and precise identification of molecular formula of small molecules, with some characterization of sub structures, without a cumbersome process of compound isolation.

Application of HRMS and LC-MS/MS techniques for qualitative and quantitative study of bioactive phytoconstituents in Indian Medicinal Plants/parts/products with their variations and identification of makers will be discussed during the seminar.

IL-27

Adenosine Receptors and Inflammation in Neurodegenerative Disorders

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The ubiquitous tissue distribution of adenosine receptors is largely responsible for the broad variety of effects produced by adenosine throughout several organ systems. Adenosine receptors are G coupled receptors and are expressed in a variety of cells and tissues making them an interesting target for the pharmacological intervention in many pathophysiological conditions like as cancer, cardiovascular disease, Alzheimer's disease, Parkinson's disease, Neuropathic pain, Asthma, COPD, Epilepsy disorder and various inflammatory diseases. Adenosine receptors are classified into three types, namely A_1, A_2 and A_3; the A_2 receptors are in turn sub-classified into two subtypes, $A_{2A}$and A_{2B} . However, there is a need for the specificity or significant selectivity towards individual receptor subtypes.

Studies have identified potent anti-inflammatory functions for all of the adenosine receptors on many different inflammatory cells and in various inflammatory disease processes. The potent effects of adenosine signaling on the regulation of inflammation suggest that targeting specific adenosine receptor activation or inactivation using selective agonists and antagonists could have important therapeutic implications in numerous diseases.

Although the basic science suggests that selective AR modulators have promise for numerous therapeutic applications, but in practice this goal has been elusive. Advances in understanding the role of adenosine and its receptors in physiology and pathophysiology as well as new developments in medicinal chemistry of ligands for these receptors have enabled researchers to identify potential therapeutic areas for drug development.

Our group has been working on both the synthesis of new thiazoles, thiophenes, imidazoles and their evaluation against acute, chronic inflammation, adenosine receptors ligands and cancer targeting Nf-kB & AP-1. The talk will cover the outcome of our work resulting in a number of molecules as selective A_1, A_2 A_3, $A_{2A}$and A_{2B} receptor antagonists as potential leads against Alzheimer's Disease, Parkinson's Disease etc.

IL-28

Analytical studies on standardized extract of a new chemotype of *Withania somnifera* Dunal (NMITLI 118RT+)

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Withania somnifera Dunal (Ashwagandha) an Indian medicinal plant, that finds use in many clinically proven conditions. NMITLI118RT+ signifies a standardized ethanolic extract derived from a new chemotype of *W. somnifera*'s roots and is one of the lead candidates in anti-stroke research. The present investigation aimed at development and validation of a simple isocratic RP-HPLC system for detection and estimation of Withanolide A and the analytical application of this method for stability indicating studies on NMITLI118RT+. A validated RP-HPLC method for Withanolide A (marker compound) estimation was used for quantification and fingerprinting of NMITLI118RT+. Forced degradation, isothermal stress tests, drug-excipient testing protocols and photolytic degradation studies were established as per ICH guidelines. The method developed was simple and rapid. This validated method could detect the marker at a retention time of around 6.3 mins and had a linearity range of 2-100 µg/mL, varying amounts of the said marker were estimated in 4 different batches of NMITLI118RT+. The various stability indicating studies carried out in the present investigation would be useful for formulation development and gave useful leads in defining the recommended storage conditions for NMITLI118RT+.

IL-29

Intellectual Property Rights: An Overview

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

IL-30

Population Pharmacokineticmodelingin optimizing drug development

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A new drug requires an average of 15 years and approaching a billion dollars in research and development [1]. Pharmacokinetics began as a way to characterize the disposition of a drug in the body and to reduce a concentration-time profile into a set of parameters that could be used for comparison, evaluation, and prediction. Pharmacokinetic model is the central piece of model based drug development. Scientifically, modeling "provides a systematic way of organizing data and observations of a system at the cell, tissue, organ or whole animal (human) levels" and "affords the opportunity to better understand and predict physiological phenomena" [2,3]. To fulfill the model based drug development, the very first step is usually a model establishment.

Pharmacokinetics of ormeloxifene and a CDRI candidate drug were studied and the pharmacokinetic parameters were estimated using classical and population approaches. Serumconcentration-time profile of the CDRI candidate drug was best described by a three-compartment open model whereas ormeloxifene was best described by a two-compartment open model using WinNonlin. A population pharmacokinetic model for ormeloxifene was developed using non-linear mixed effect modeling program, NONMEM. The structured model selected for ormeloxifene consisted of a submodel of a proportional linear subsystem with first order conditional estimation with interaction (FOCE-I).The model establishment using WinNonlin and NONMEM will be discussed.

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IL-31

NMR-based Metabolomics to study the tissue specificity, seasonal and geographical variations in *Alstonia scholaris*

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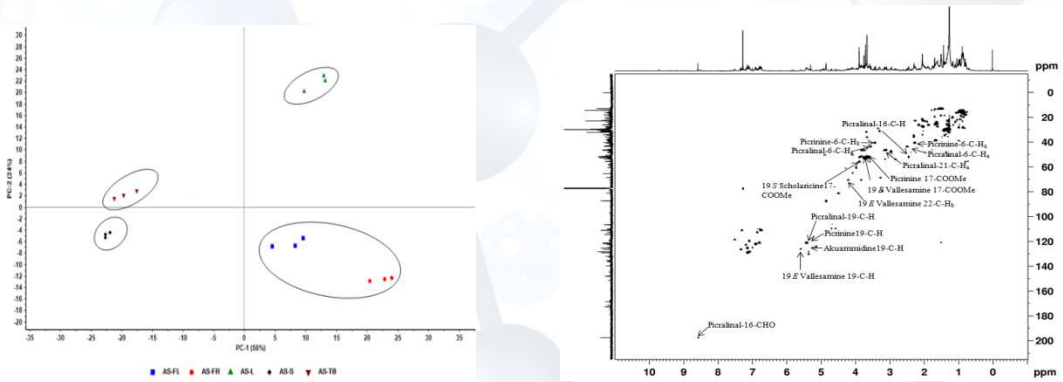
Plants have a great diversity of secondary metabolites. Their presence and production is depending upon the tissues and climatic condition of the particular region, where the plant is grown. Amongst the class of compounds present in medicinal plants, alkaloids stand as an important class of compounds for the development of new drugs. *Alstonia scholaris* is one of the richest sources of the alkaloids and there **has always been** interest among the scientist to utilize this class of compounds from this plant for therapeutic purposes. The NMR spectroscopy and PCA method have been applied for metabolic profiling of several kinds of wine, coffee, juices, beers and some plants.[1,2] The first objective of the present study was to identify/characterize the alkaloids in different parts of this plant. The other objectives were the tissue specific metabolic profiling of the identified alkaloids in trunk bark, stem, leaf, flower and fruit as well as geographical and season specific metabolic profiling of alkaloids. Various one and two dimensional NMR experiments were utilized for the characterization of the alkaloids. Alkaloids have been successfully characterized and quantified.[3] NMR spectroscopy coupled with the Principal Component Analysis (PCA) and **Partial Least Squares Discriminant Analysis (PLS-DA)** was utilized for the targeted secondary metabolic profiling. NMR and multivariate analysis clearly indicate that there are variations in presence and amount of alkaloids in different parts of *Alstonia scholaris* as well as due to seasonal and geographical changes. Qualitative and quantitative analysis of metabolites of the medicinally important plants may provide information regarding when and which part of plant should be collected to obtain substantial bioactive ingredients for desirable pharmacological activity. This study will also provide a complementary tool for quality control of herbal medicinal products when these plants are used.



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IL-32

Stereoselective Syntheses of Naturally Occurring 20-epi Cholanic Acid Derivatives and Other Bioactive Compounds From 16-Dehydropregnenolone Acetate

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A wide variety of diterpenes, sesquiterpenes and steroids have been reported to have modified isooctyl (cholesterol-type) side chains and the unit being attached to the polycyclic nucleus at C-17 with (R) or (S) stereochemistry at C-20. The introduction of the properly functionalized side chains onto tetracyclic steroidal starting materials has been the subject matter of several investigations. An important problem that arises in this approach is the stereoselective control of the C-20 stereochemistry. These efforts have been spurred by the biological significance of new natural products containing modified side chains and synthetic endeavors towards a variety of vitamin D metabolites, brassinosteroids, squalamine, OSW-1, ent-steroids and various marine steroids.

We have reported the synthesis of C(20R) aldehydes by ionic hydrogenation of C-20, 22-ketene dithioacetal and C-20 tertiary alcohols with 100% stereoselectivity. In addition to this, we would like to discuss the stereoselective syntheses and ionic hydrogenation of various steroidal C-20 tertiary alcohols to the corresponding steroid derivatives with natural and unnatural configuration at C-20. Elaboration of the synthesized intermediates to biologically active compounds will be discussed.

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IL-33

Indole derivatives and indole based alkaloids from dithiocarboxylates

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Among the heterocyclic compounds, the indole scaffold is a prominent and privileged structural motif found in numerous natural products such as the neurotransmitter serotonin, anticancer agents like vinblastine, mitomycin C, and the antihypertensive alkaloid reserpine. Also, a number of important synthetic drugs such as sumatriptan, tadalafil, rizatriptan and fluvastatin contain indole motifs. Due to their remarkable pharmacological and therapeutic activities the synthetic methodologies of indoles have attracted considerable attention from chemists. In this conference some of our research findings using dithiocarboxylates [1] on the novel synthetic methods of indole based fused heterocycles and certain indole alkaloids will be disclosed [2].

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IL-34

Invention of A New Male Antifertility Injection- RISUG in India for 21st Century

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Population explosion is a worldwide problem in present scenario. India takes second position in world in view of population, so this is a thinkable topic for the entire reproductive biologist. They develop new contraceptive methods that are cost effective and easily available.

Prof. S. K. Guha is a well known renowned biomedical engineer who established biomedical engineering department at AIIMS and IIT, Delhi. He developed a new male antifertility injection - RISUG (Reversible inhibition of sperm under guidance) which is a synthetic polymer styrene maleic anhydride (SMA). RISUG injection when given in the both vas-deferens of males , formed a blockage in the vas-deferens and prevent the passage of sperm f through vas-deferens and worked as male contraceptive. The special advantage of this injection is reversibility of the fertility. When required the vas deferens is flushed with another injection of dimethyl sulfoxide or sodium bicarbonate solution. RISUG is only single injection that has reversible contraceptive activity.

At our institute in toxicology division, the preclinical toxicity studies were done in rats , mice, rabbits and rhesus monkeys by my group in which the compound was found safe. At present, the compound is in phase-III clinical trial stage. The study protocol, plan of experiments and results of preclinical toxicity studies will be presented and discussed in the conference.

IL-35

Functionalized Heterocycles: Scope & Applications

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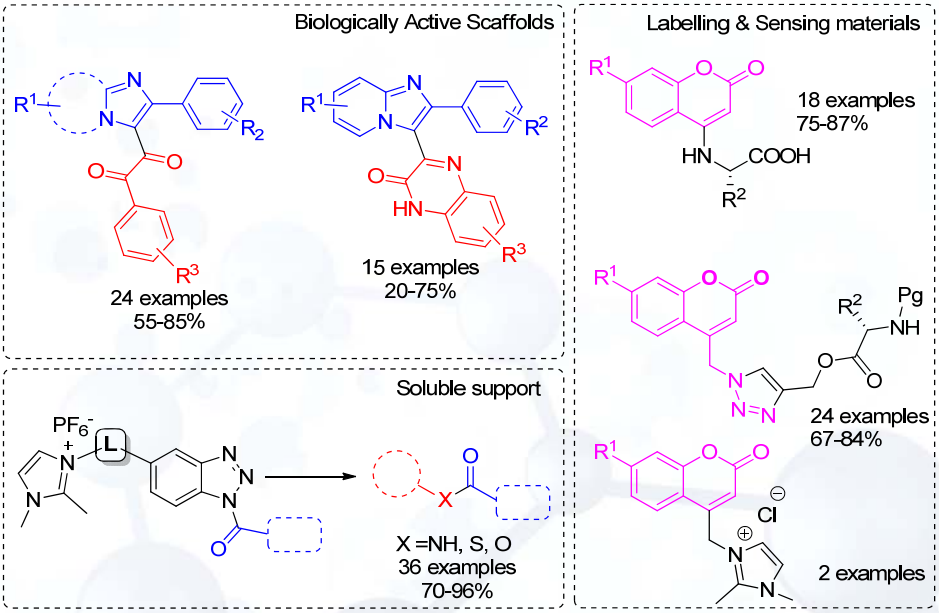
Development of effective methods for the construction of heterocyclic scaffolds remains a challenging task in organic chemistry. Cycloaddition, cross-coupling, and C-H activation/functionalization reactions are powerful tools for the construction of diverse array of functionalized heterocycles of medicinal and pharmaceutical importance. In addition, developing methodologies in a greener fashion either by eliminating solvents or using relatively benign solvents such as water, ionic liquid for the synthesis and applications of chemical entities is on high demand, considering environmental inverubilty.[1] In regard to these aspects, some recent results[2-8] on the development functionalized heterocycles and their applications (Figure 1) will be discussed.



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IL-36

Design, synthesis and application of N-glycoconjugates as multi targeting drugs

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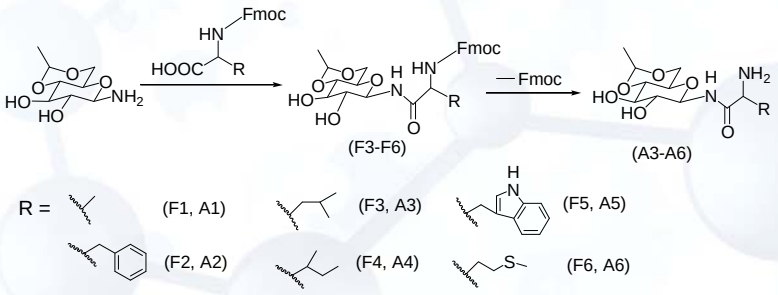
The carbohydrates are one of the major energy sources for living organisms and are required in the formation of polysaccharides, nucleic acids and antibiotics. It's association with protein acts as hormones, protective agents, structural molecules etc. Glycopeptides are well known for its antibiotic and antibacterial activities, while salicylic acid derivatives are used as anti-inflammatory and analgesic agent. With this literature background, we are exploring the activities of new compounds developed by combining the different chemical entities having pharmaceutical importance, which might act as multi targeting drugs. Developing the multi targeting drugs are one of the prime requirements of the current era as single targeting drugs might not always affect the complex systems in desired way. In this direction, Glucopyranosylamine has been condensed with amino acids and the resultant compounds have been tested for antibacterial activities. Six glycoconjugates (A1-A6; Scheme 1) were tested against G(+)ve (*Bacillus cereus (B. cereus)* and G(-)ve (*Escherichia coli* (*E. coli)* and *Klebsiella pneumoniae (K. pneumoniae*) bacterial strains and all the compounds exhibited moderate to significant antibacterial activities [1].

Further, one these compounds (A1) were coupled with salicylic acid derivatives via amide linkages and resultant salicylamide derivatives were tested for anti-inflammatory and analgesic behavior. Anti-inflammatory studies were performed using carrageenan-induced rat paw oedema model, while acetic acid-induced writhing test model was adopted for analgesic studies. All the tested compounds exhibited fair amount of both, anti-inflammatory and analgesic behaviors [2].



Scheme 1

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IL-37

Conformational control due to Arene interactions in Flexible Pyrazolo[3,4-*d*]pyrimidine core Based Models

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Pyrazolo[3,4-*d*]pyrimidine which is isomeric with biologically important purine system will be used to demonstrate conformational control, both in solution and solid state, due to arene interactions in flexible compounds based on propylene (trimethylene) butylidene and ethylene linkers. Study will be extended to other arenes like purine, triazolo[4,5-*d*]pyrimidine, pyrrolo[2,3-*d*]pyrimidine, phthalazinone, quinazolinone, etc. for determining the scope of such conformational control. Substituent and steric effects will also be studied in such unusual conformational control.

IL-38

Are flavonoids a possible source of new cardiovascular drugs?

Přemysl Mladěnka

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Flavonoids are a large group of compounds with many suggested cardiovascular effects. However, although many epidemiological studies found a relationship between intake of flavonoids and cardiovascular diseases, clinical evidence of positive cardiovascular effects of flavonoids is sparse. Moreover, structural diversity of flavonoids and their complex metabolism seem to be important determinants for their effects. This lecture willsummarize the possible mechanisms of action of flavonoids relevant to the cardiovascular system. Emphasis will be given on the structure/activity relationship and possible clinical relevance.

IL-39

Multiscale Approach to Drug designing and Challenges for Next Millennium

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Scientifically and technologically important materials can be found in all shapes and sizes. In fact, they can range from molecules to complex composites and mixtures. Depending upon the spatial dimensions of the system and properties under investigation, computer modeling of such materials can vary from quantum mechanics to classical force field molecular mechanics and dynamics, from *ab-initio* Quantum molecular dynamics to Monte Carlo simulations to mesoscale simulation etc. Due to broad range of relevant system sizes and timescales and in the light of emerging trends in modern computational science, the need of the hour is to adopt so called Multiscale modeling for the problem at hand. In this presentation, I will discuss some results obtained by applying Multiscale modeling techniques in describing biological properties of wide range of molecules/materials. With Multiscale modeling, we combine methods on many different length and time scales in order to obtain a more complete understanding of the system under study. The combination can be obtained in terms of either integrated algorithms or simply by piping datasets from one model to another. The part of presentation will also highlight the need and difficulties in computer modeling approach and the way forward looking into future of drug designing.

IL-40

Aminocatalyzed Transformations of Dicarbonyls: Asymmetric Synthesis of Medium Sized Nitrogen Heterocycles

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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 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 as SMNPs will be presented here.

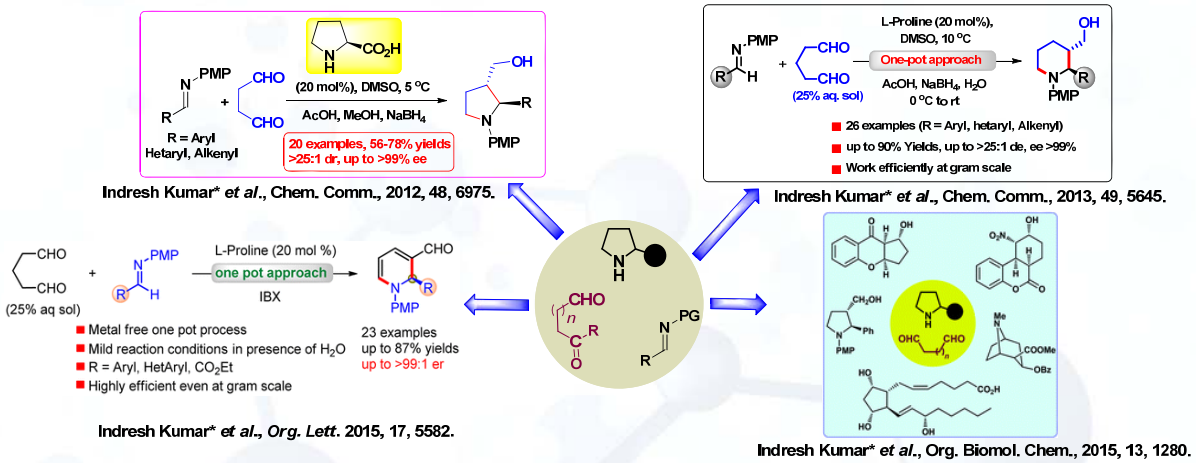

Figure 1: D-A annulation approaches for the asymmetric synthesis of SMNPs

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IL-41

Greener and efficient approaches for the syntheses of biologically potent scaffolds

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

Our group has been working since more than a decade on the development of novel and efficient methodologies for the synthesis of structurally diverse biologically active compounds. In the present talk, I would like to emphasize some of our novel and efficient synthetic strategies for the synthesis of carbamates, dithiocarbamates, xanthates, dialkyl carbonates, *S,S*-dialkyl dithiocarbonates, trithiocarbonates, substituted ureas, α-amino nitriles, and substituted *N*-aryl lactams *etc* employing cheap and safe alternatives starting from a variety of starting materials, reagents and catalytic systems.

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IL-42

Organoiodine reagents in the construction bioactive heterocycles

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In recent years, organoiodine reagents have emerged as versatile and environmentally benign reagents for the construction of numerous nitrogen containing heterocycles [1]. The advent of organoiodine reagents has provided a range of organic transformations such as oxidations, oxidative cyclizations, carbon-carbon and carbon-heteroatom bond formations and C-H functionalizations under mild reaction conditions [2]. Moreover, these reagents can be easily accessible from the readily available starting materials. Owing to the reduced toxicity, recyclability and easy handling, these reagents are better alternative to some of transition-metals utilized in organic transformations. Among the various organoiodine reagents, few prominent reagents, namely (diacetoxyiodo)benzene, hydroxy(tosyloxy)iodobenzene and diaryliodonium salts got plethora of applications in organic and medicinal chemistry [3]. The resurgent of interest in organoiodine reagents led to discover new iodine reagents and novel synthetic routes for the construction of useful bioactive molecules. On the other hand, heterocyclic compounds are privileged scaffolds comprised in many valuable natural and pharmaceutical agents so there has been continuous interest to construct these kinds of medicinally important molecules under mild reaction conditions [4]. Inspired by the remarkable advantages of organoiodine reagents and quest towards the development of novel synthetic routes, recently, we have achieved diverse naturally and synthetic bioactive heterocycles by employing organoiodine reagents [5]. Synthesis of various azaheterocycles and their interesting biological properties will be discussed in the presentation.

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IL-43

C/N-Arylation Chemistry: Development of Synthetic Tools for Medicinal Chemist

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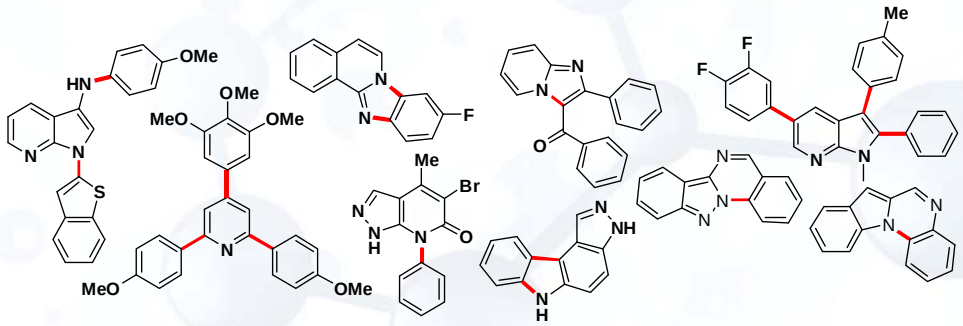
The drug discovery industry remains solely reliant on synthetic chemistry methodology to prepare compounds for small-molecule drug discovery program. The expansion of synthetic methodology in recent years has greatly facilitated the preparation of molecules that would once have been considered an insurmountable synthetic challenge. In turn, the drug discovery industry, where large numbers of molecules are prepared and tested as potential new medicines is one of the principal end-users and beneficiaries of this enlarged toolkit. Industrial medicinal chemistry departments the world over are charged with the rapid delivery of small molecule new chemical entities (NCEs) into the screening process to facilitate the discovery of novel medicines to allow for the prevention, management or cure of disease. While this headline aim seems straightforward on paper, the reliable, timely and dependable synthesis of NCEs remains an unpredictable art that calls for the application of robust and reliable chemical transformations to best ensure chances of success and to help alleviate the bottlenecks often caused by synthetic tractability issues within a drug discovery program. It is little wonder that chemists have therefore developed a repertoire of transformations that to a greater or lesser extent can be relied upon to furnish the desired derivatives across a variety of pharmacophores generated *via* structure activity relationship (SAR) study. In this aspect there is always a high demand for new methods to facilitate the formation of C/N-aryl bonds as they are common motif in pharmaceutical designed compounds. Designing and discussing of various synthetic tools (C/N-arylation) for the use of medicinal chemistry and generation of new chemotypes will form the basic premise of my presentation.[1]



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IL-44

Targeting DNA Damage/ Repair pathways: Towards Novel therapeutics for cancer

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Cancer is one of the leading causes of death worldwide. Several cases chemotherapy becomes ineffective by the upsurge of resistance and toxic. The talk would give a brief idea of a systematic way to target cancer by choosing the right targets involved in cancer cell signaling. One of the pathways that our group is looking is DNA repair mechanism especially the pathways involved in ATR signaling. Can ATR be targeted for cancer therapy? This would be question that we would like to answer by developing small molecules to study the mechanism and eventually develop novel therapeutics.

IL-45

Locating evasive patents of process/technologies & importance of indexed databases

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Finding information is easy and in fact, we struggle with too much information today. However hunting for relevant and precise information is challenging and the fear of missing important competitive technologies/data makes locating information even more challenging.

Patents pose a challenge since it is written in techno-legal language with an aim of masking the actual technology to the extent that simple chemistry/bio concepts are at times difficult to decipher. Hence, domain expertise is needed to index the substances/concepts/processes in a structured way so that it becomes easy for users to locate relevant information quickly. Chemical Abstract Service (CAS) databases powered by this value added indexing in tandem with ability to upload structures/reactions/biosequence codes etc. This helps you find the evasive technologies which are critical for research related decisions.

We would present cases discussing tricky situations of incompletely defined and manually registered substances/compositions, prophetics, chemically modified or post processed macromolecules and various database supported classification systems to quickly locate relevant information.

IL-46

Songhui Wang

China

Abstract Awaited

ORAL

O-1

Amino acid ester analogs as cardiac CASQ2 depolymerization inhibitor

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Cardiac calsequestrin (CASQ2) undergoes Ca^{2+}-induced dynamic polymerization and this property is significantly impaired by catecholaminergic polymorphic ventricular tachycardia (CPVT) mutations. Different classes of small molecules have been suggested to bind to CASQ2 on the basis of docking, X-ray crystallography, biological studies and affect its polymerization pattern. However, many of them were found to be cardio-toxic. We explored the possibility of regulating CASQ2 polymerization by amino acid ester analogs (**3a-t**) through evaluation of their potential to inhibit depolymerization of CASQ2. Compounds **3e** and **3m** were able to inhibit more than 50% CASQ2 depolymerization at 100 nM and 250 nM respectively. This is the first *in-vitro* biochemical evaluation report of small molecules with ability to stabilize CASQ2 polymers and opens up possibility of fixing Ca^{2+}-release disorders by targeting CASQ2.

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O-2

DEVELOPMENT OF VITAMIN E-DERIVATIVES AS AKT INHIBITORS & ANTICANCER AGENTS

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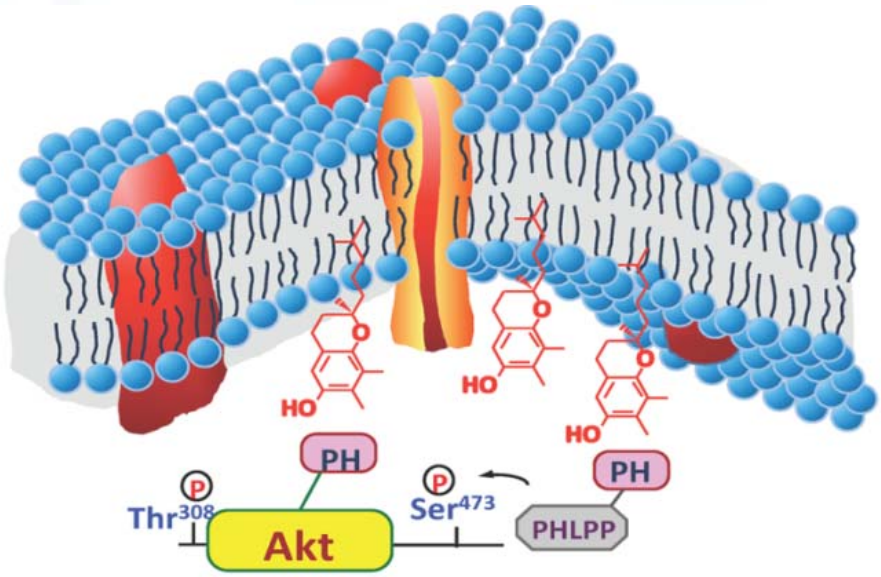
Abstract: Recently Akt represented a unique target for the PTEN-negative prostate cancer. In the current study a series of vitamin E derivatives has been prepared and evaluated for their antitumor efficacy against PTEN-negative prostate cancer. Several of these derivatives showed remarkable antitumor activity. After lead optimization it was found that compound 3 & 20 preferentially recognized the PH domains of Akt and PHLPP1. Moreover, compound 20 was orally active in suppressing xenograft tumor growth in nude mice. This finding provides a basis for exploiting a novel class of PHLPP1-targeted Akt inhibitors in PTEN-deficient cancers.



O-3

Synthesis of sulfoxide from sulfide using Plant Peroxidase

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Abstract: Enantiomerically pure sulfoxides are important synthons for the asymmetric synthesis of natural products and rank among the most powerful stereodirecting groups. For these reasons numerous studies have been devoted at chemical methodologies leading to this structural unit and good to excellent stereoselectivities have been reported for the oxidation of organic sulfides to the corresponding sulfoxides[1]. Many sulfoxides and sulfones are used as versatile intermediates for various organic transformations[2]. Additionally, these compounds have been proved to be active pharmaceutical ingredients for several therapeutic drug molecules.[3] Sulfoxidation of organic sulfides is a straight forward method for the selective preparation of sulfoxides or sulfones.

Chloroperoxidase is a heme protein possessing several diverse catalytic abilities. Very recently it has been used in the peroxide dependent enantioselective oxidation of organic sulfides to the corresponding sufoxide.[4] However, Chloroperoxidase from *Cladario fumago*, a marine fungus, only has been used so far this purpose. This communication reports a crude preparation of Chloroperoxidase from *Musa paradisiaca* which can be conveniently prepared and used for the transformation of phenyl methyl sulfide to its sulfoxide. This is the first report of sulfoxide formation using a plant chloroperoxidase.

The method for the preparation of chloroperoxidase from the stem of *Musa paradisiaca* has been developed. The enzymatic characteristics like Km for the substrates phenyl methyl sulfide and H_2O_2, pH and temperature optima of the enzyme have been determined. The enzymatic transformation of phenyl methyl sulfide to its sulfoxide has been demonstrated. The effect of hydrogen peroxide on sulfoxidation of thioanisole has been studied. The results of the above studies will be presented in the conference.

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O-4

Visible Light Catalyzed Photooxidative Heterocyclization of Semicarbazones for the Synthesis of 1,3,4-Oxadiazoles

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The development of green methods for the formation of C-C and C-N bonds is of great importance and remains a pre-eminent goal in current synthetic chemistry.[1] In this venture, photocatalysis using visible light represents a unique strategy because of its inherent green chemistry features.[2]. In requisite of a cheap, ecofriendly and metal-free catalyst, an organic dye eosin Y has pledged to be indispensable for high photocatalytic performances.[3]

Among five-membered heterocyclic compounds, 2,5-disubstituted 1,3,4-oxadiazoles have become an important construction motif for the development of new drugs. Several methods are reported in the literature utilized reagent require special care for handling and are not eco-compatible.[4] The work-up procedure for each synthetic step to yield desired products requires great precautions. Hence, the development of simple, efficient and ecofreindly methods for the rapid and concise synthesis and modification of oxadiazole motif need to be developed.[5]

Therefore, we have developed an efficient, metal free and direct pathway for a one-pot synthesis of 2-amino-5-aryl-1,3,4-oxadiazoles under mild conditions. The protocol involves the visible light mediated intramolecular, aerobic oxidative heterocyclization of substituted semicarbazones to 1,3,4-oxadiazoles using CBr_4 as an oxidant and eosin Y as the photoredox catalyst. This protocol is a superior alternative to the existing syntheses of 1,3,4-oxadiazoles with the advantage of employing visible light and atmospheric oxygen as the greenest and sustainable reagents.

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O-5

Plant Derived Lead Molecules as Pharmacologically Active Agents

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Structurally diverse and pharmacologically active natural products isolated from plants, animals and microorganisms have proven to be effective drugs since many years and have made important impact on curing dreadful diseases. The discovery of pure compounds as active principles in plants was first described at the beginning of the 19thcentury, and the art of exploiting natural products has become part of drug discovery research. The discovery of quinine from *Cinchona succiruba* and its subsequent development as an antimalarial drug represented a milestone in the history of antiparasitic drugs from nature for the treatment of parasitic diseases, artemisinin isolated *Artemisia annua* and its derivatives artemether and artesunate are most effective antimalerial drugs against multidrug resistant *P.falciparum* and pencillins, streptomycins and tetracyclines used as antibiotics. Moreover, plants derived anticancer agents, viz. vinblastine, vincristine, camptothecin, topotecan, etoposide and texol played significant role and effective against the verities of cancer cell lines, In the continuation of our work to isolate and identify the lead molecules from traditional medicinal plants by bioassay guided fractionation, we have identified the active constituent having antigiardial activity from *Phlebophyllum* kunthianum[1], antimicotic anthraqinones from *S. fragran*s[2], and spirostan saponins from *A. africanus*[3]as antidermatophytic agents. The recent developments on the discovery of pharmacologically active lead molecules from plants including our finding will be discussed during presentation.

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O-6

DESIGN OF 2-SUBSTITUTED BENZIMIDAZOLE DERIVATIVES AS PROCASPASE-3 ACTIVATORS AND APOPTOSIS INDUCER: 3D QSAR, DOCKING AND *IN SILICO* ADMET STUDY

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Nowadays, the goal of cancer therapy has shifted to target the magic bullets, which can induce apoptosis in the cancer cells. Procaspase-3 is one such magic bullet for the induction of apoptosis via activation of caspase 3. In this study, 3D QSAR study was performed on benzothiazole derivatives bearing the *ortho*-hydroxy-*N*-carbamoylhydrazone moiety. Three different alignments were used (rigid body, pharmacophore and docking-based) for CoMFA and CoMSIA analysis. The best QSAR models were obtained using rigid body alignment method (Distill). CoMFA and CoMSIA models were found statistically significant. Generated QSAR models were utilised for the design of novel compounds. Docking study was performed with designed compound to predict both ligand orientation and binding affinity. Activity of designed compounds was predicted using generated CoMFA and CoMSIA models. *In silico* pharmacokinetic properties and toxicities were predicted using osiris property explorer and Med Chem Designer software. The present molecular modeling approach along with structure-based technique and ADMET prediction provides useful information for the design of novel 2-substituted benzimidazole derivatives with better selectivity and efficacy.

O-7

Design, Synthesis and Anti-HIV Activity of Novel Quinoxaline Derivatives

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Abstract: Acquired immune-deficiency syndrome (AIDS) is a fatal condition developed due to infection of human immunodeficiency virus (HIV).[1] The infection with HIV virus weakens body's defence system and hence, person becomes susceptible to various infections.[2] Drug resistance due to development of resistance virus is another major drawback of available anti-HIV drugs.[3,4] Hence, there is a urgent need to develop more efficient anti-HIV agents. With the aim to find novel HIV inhibitors, two ligand based drug design approaches: pharmacophore modelling and 3D-QSAR study were used initially. The information obtained through both approaches in form of features of pharmacophore model, hits of virtual screening and 3D-QSAR contour maps [5] were used to design novel anti-HIV agents. Designed compounds were then docked into the active site of HIV-1 integrase enzyme. Few designed compounds showed interactions with DDE loop amino acids, chelates Mg^{2+} ion in an active site and interacts with amino acids whose mutation causes development of resistance. Best docked compounds were selected for synthesis on the basis of their docking scores and interactions. After planning of synthetic scheme, actual synthesis was carried out. Spectral characterization of final synthesized compounds **7a-7g** was carried out using FTIR, ^{1}H & ^{13}C-NMR and mass analysis. % purity of compounds were checked using HPLC. Seven characterized compounds were then subjected to anti-HIV activity [6] and cytotoxicity study. Compound **7d** and **7e** showed better anti-HIV activity than other derivatives and also found non-cytotoxic, hence can be considered as novel hits to develop more potential HIV inhibitors.

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O-8

Unexpected functional implication of a stable succinimide: a novel mechanism for structural stability in *Methanocaldococcus jannaschii glutaminase* (MjGATase)

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Succinimide intermediates are transiently formed during deamidation of asparaginyl or dehydration of aspartyl residues in peptides and proteins. Rapid hydrolysis of this intermediate to aspartyl and iso-aspartyl residue and, the resultant accumulation of the latter are generally associated with loss of protein structure and function[1–3]. Contrary to this dictum, we report the existence of a remarkably stable succinimide, which is resistant to hydrolysis at high temperatures (up to 100 °C), high concentration of chaotrope (8 M GdmCl) and to low pH. Further, we for the time, ascribe a functional role for this post-translational modification in imparting structural stability to the glutaminase subunit of GMP synthetase from a hyperthermophilic archaeon *Methanocaldococcus jannaschii*. The enzyme harbouring succinimide remains completely soluble and fully functional up to 100 °C and retains its well folded structure even in 8 M guanidinium chloride (GdmCl). However, mutants lacking the succinimide fail to retain their structure above 85 °C or in 4-5 M of GdmCl. Our findings suggest that protein sequences that spontaneously form and stabilize succinimide; a side-chain- backbone cyclization that reduces conformational flexibility, may serve as a potential mechanism for structural stability at high temperature.

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O-9

A novel, facile, rapid protocol for the one pot green synthesis of imidazoheterocyclicscaffolds viathree component condensation reactions

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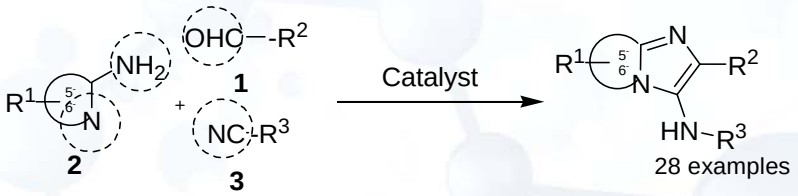
The imidazohetrocyclic scaffolds one of the most important fused heterocyclic compounds, are attractive for drug discovery, since many compounds incorporating these scaffolds exhibit a wide range of biological, medicinal, and pharmaceutical activities, such as antitumor, anti-inflammatory, antiviral, antiprotozoal, anticonvulsant, anxiolytic, hypnotic, gastrointestinal, antiulcer, and immunomodulatory activities.[1,2] Furthermore, imidazohetrocyclic scaffold forms the core structure of several drug molecules like zolpidem used in the treatment of insomnia, alpidem, as an anxiolytic agent, olprinone for the treatment of acute heart failure, minodronic acid useful for the treatment of osteoporosis, and zolimidine used for the treatment of peptic ulcer.[3,4]In this regard, development of easier and effective synthetic methods, as well as new derivatives with this structure, is important in organic synthesis. Although several methods have been reported for the synthesis of imidazohetrocyclic scaffold, many of these methods are based on multi-step syntheses, and the range of compounds that can be prepared is limited. In this paper, we synthesized some new derivatives having imidazohetrocyclic scaffolds as core structure via Groebke-Blackburn-Bienayme (GBB) reaction disclosed independently in 1998 by three research groups.[5]In this reaction, pyrazole substituted aldehyde (1), 2-aminoazine and an isonitrile reacted in presence of suitable catalyst to afford a highly substituted imidazole derivatives (Scheme).



Scheme: Synthesis of theimidazohetrocyclic scaffolds based derivatives

References:

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O-10

Chiral Cobalt(III) Complexes: Hydrogen Bond Donor Catalysts for Enantioselective Organic Synthesis

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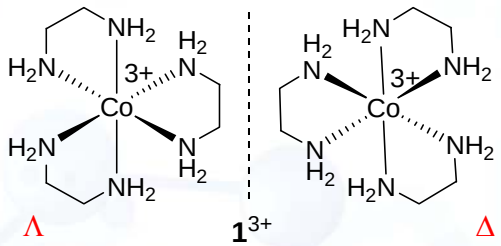
Hydrogen bond donor catalysis for asymmetric synthesis have witnessed an extensive development in recent years. [1] Recently a new family of inexpensive and readily available chiral hydrogen bond donor catalysts based on Cobalt (III) Werner complexes for which the trication $[Co(en)_3)]^{3+}$ ($\mathbf{1}^{3+}$) is the prototype. [2] The mirror images of $\mathbf{1}^{3+}$, depicted in Scheme 1 are commonly designated and . Salts of these trications were among the first inorganic compounds separated into enantiomers. [3] These salts have been successfully used for enantioselective organic synthesis. [3] In order to established the broad synthetic utility of these salts, we have synthesized new lipophilic chiral Werner salts and investigated these for new reactions which will be will be presented.



Scheme 1

References:

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O-11

Convenient synthesis of Green/Cyan Fluorescent Proteins Chromophoreusing Amino acids

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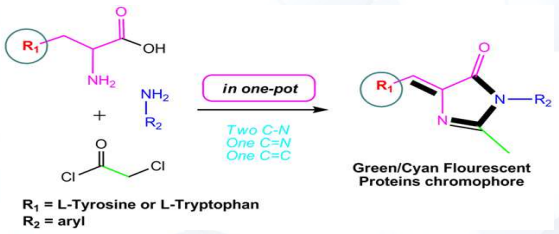
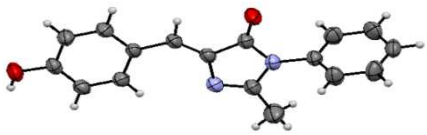
Nitrogen containing heterocycles are of special interest in synthetic organic chemistry, since they occur in a wide variety of natural products. Among them, imidazolinone is a fundamental non-aromatic naturally-occurring heterocycle that has been intensively used in the synthesis of functional materials and pharmaceuticals.[1]The imidazolinone substructures are found to act as the chromophores of the fluorescent proteins (FPs), for example, green fluorescent protein (GFP), cyan fluorescent protein (CFP), blue fluorescent protein (BFP) andfor red kaede fluorescent protein (RFP).[2]Imidazolones also show various biological and pharmaceutical activities. The omnipresent of 4-arylidene-5-imidazolinones and their intrinsic photochemical phenomena have made it intriguing synthetic targets and useful chemical models for investigating the mechanism of the fluorescence proteins.[3]

Herein, we report a new phosphorous-catalyzed tandem approach for the synthesis of 4-arylidene-5-imidazolinones (4/5a-i), which are Green FPs and Cyan FPs chromophore respectively.The reaction involve assembly of *N*-chloroacetyl-amino acids (1a'/b') and anilines (3), wherein (1a'/b') are generated *in situ* by the direct use of the corresponding aromatic amino acids (1) and acyl chlorides (2) in one pot (Scheme 1).





Scheme 1. Synthesis of 4-arylidene-5-imidazolinones 4a

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O-12

*De-Novo*lead optimization of potent Plasmodium falciparum phosphoethanolamine methyltransferase inhibitors

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Malaria is one of theleading source of childhood mortalitycaused by parasitic infection, but the disease control efforts are threatened by resistance of the plasmodium parasites to current therapies.Intense research efforts are focused on identification of new potent antimalarials. We report here, a structure based drug discovery strategy for design and synthesis of a series of potent and novel triazine based antimalarials. The X-ray structure of *Plasmodium falciparum*phosphoethanolamine methyltransferase (*Pf*PMT) is used as a target as it is unique to the parasite. Trisubstitutedtriazine and its anlaogs are produced by an inexpensive three to four step synthesis giving excellent yields. Parasite growth inhibition assays further confirmed the activity of the molecules to be in 5 to 0.8 µM range showing selectivity towards the parasite over mammalian cells. Molecular dynamics simulations on the *Pf*PMT-inhibitor complex shed light on the inhibition mechanism for further optimization of the lead compounds.

O-13

Development and in vitro-in vivo evaluation of hollow gastro retentive microspheres of an anti-diabetic drug prepared by emulsification solvent evaporation method

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Hollow microspheres were prepared for the drug glipizide by solvent evaporation emulsification method using water permeable polymer, cellulose acetate. A floating depot forming oral dosage formulation was prepared to prolong the residence of the drug in GIT. Formulations were optimized *in vitro* for physicochemical characteristics and drug release. The microspheres exhibited good encapsulation efficiencies and micrometric properties. The microspheres had low density and may be retained in the stomach environment for long durations (buoyant over gastric juice for over 10 hrs). The prepared microspheres exhibited prolonged drug release. The release rate decreased and the mean particle size increased at higher polymer concentrations[1]. Stirring speed affected the morphology of the microspheres and revealed that, the biocompatible depot-forming polymeric microspheres controlled the drug release [2] as shown in figure 1. *In vivo* studies were carried out in male albino mice by studying the hypoglycemic effect of the formulation on oral administration to normal and alloxan-induced hyperglycemic mice and was found to be sustained for over 10 hrs with the formulation as compared to the pure drug. The plasma glucose lowering effect was seen; the maximum lowering of the glucose level was seen at 4.5 hours with reduction of about 25 % in hyperglycemic mice [Fig 2]. The pharmacokinetic parameters of the drug were also found to be altered with significant changes in elimination half life of drug, AUC, Cmax and tmax. These formulations, with their reduced frequency of administration and better control over drug disposition, may provide an economic viable to the user compared to products currently available for diabetes control.

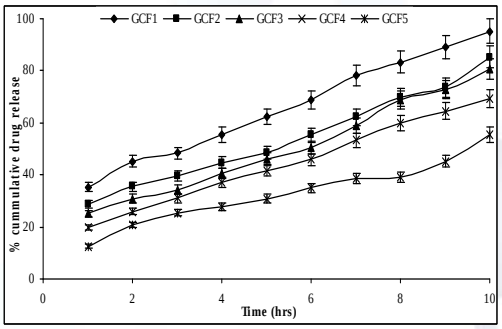

Fig1. In vitro drug release

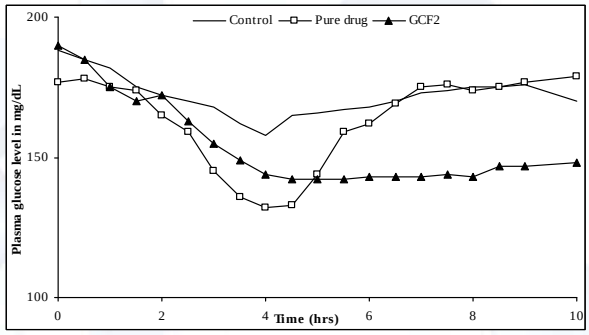

Fig2. Plasma glucose level reduction in mice

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O-14

4-[2-(5-Ethylpyridin-2-yl)ethoxy]benzaldehyde and its analogs: A useful pharmacophore for antibacterial, antifungal and antitubercular agent

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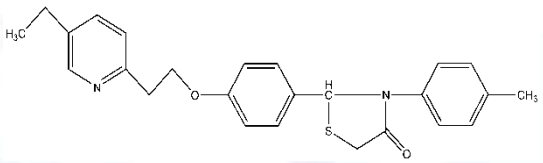
Abstract: Medicinal chemistry is an enhancing branch of science, which has remarkable value for synthesis of novel drugs with intense therapeutic activity. It concerns with discovery, development, identification and interpretation of mode of action of biologically active compounds at molecular level. In the field of science and technology, medicinal chemistry has been considered as a fascinating subject. The rapid development in the last several decades has been truly a challenging and very exciting. 4-[2-(5-Ethylpyridin-2-yl)ethoxy]benzaldehyde[1] is a leading active metabolite, which is one of the key intermediate to pioglitazone, a well known pharmaceutically active compound and used as an insulin sensitizing agent in the treatment of diabetes. Moreover 4-[2-(5-ethylpyridin-2-yl)ethoxy]benzaldehyde, which combines with 2,4- thiazolidinone gives an antidiabatic activity. Chalcones[2,3], pyrimidines[4], Schiff bases, thiazolidinones and azetidinones[5] are medicinally efficient entities. Looking to the importance of 4-[2-(5-ethylpyridin-2-yl) ethoxy]benzaldehyde, we have generated newer analogs viz, chalcones, pyrimidines, Schiff bases, thiazolidinones and azetidinones for their antibacterial, antifungal and antitubercular activities.



Keywords: Chalcone, Pyrimidine, Schiff base, thiazolidinone, azetidinone, antitubercular, antibacterial, antifungal activities

References:

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O-15

Design & Development of therapy for Prostate Cancer based on Synthetic & Semi synthetic molecules

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Abstract: Prostate cancer (PCa) is the most often diagnosed noncutaneous tumor and the second leading cause of cancer deaths among men in U.S respectively. Androgen receptor (AR) is a DNA-binding transcription factor, belonging to nuclear receptor subfamily, which regulates gene expression. Androgen deprivation therapies are front-line treatments, in addition to surgery and radiotherapy in patients with advanced disease. Current chemotherapeutic agents include abiraterone, cabazitaxel, and enzalutamide (MDV 3100) have emerged for CRPC patients.[1] 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 to the clinical management of this cancer. Therefore, the modification of existing drugs and evolution of specific targeted therapeutics are currently carried out to minimize the toxicity, minimizing drug resistance and lowering therapeutic doses.

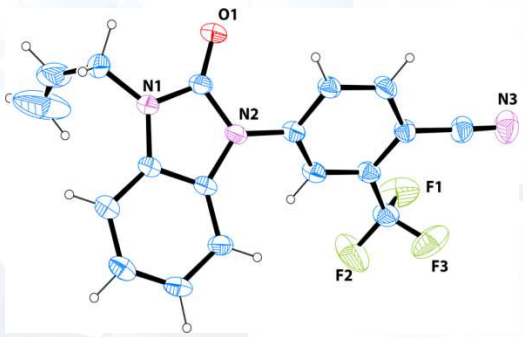

Fig.1 An ORTEP representation of the compound

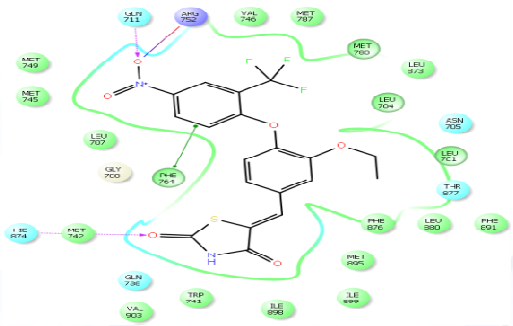

Fig.2Predicted binding mode of the compound in the AR crystal structure.(2AXA)

Taking into account the interesting properties of these benzimidazole & 1, 3-thiazolidine-2, 4-dione derivatives and in continuation of our research, we designed and synthesized novel molecules and the in vitro antioxidant and anti-prostate cancer activities were also evaluated.[2] Further, the structures were confirmed by single crystal XRD analysis.[3,4] AR protein character and binding site were studied in details using Schrödinger software. The best fit new chemical entities (NCEs) were synthesized in the wet lab. In order to investigate their anticancer activities, all NCEs were tested against prostate cancer cell lines (PC-3, LNCaP). Bicalutamide were used as reference drugs. ADME/T properties and DFT calculations were predicted for those compounds. Clearly, these lead compounds may be used for the development of anti-prostate cancer agents.

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O-16

Synthesis of Fluoro Analogue of Neplanocine A: Their Antiviral and Antitumor Activities

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Abstract: NeplanocinA (NPA) **1**, isolated from *Asperillusniger* is one of the representative carbocyclic nucleosides that exhibit wide spectrum of antiviral and anticancer activity.

NPA inhibits *S*-adenosyl-L-homocysteine (SAH) hydrolase, which effects cleavage of S-adenosyl-L-homocystein (SAH) to adenosine and L-homocysteine. SAH is the product of S-adenosyl-L-methionine (SAM)-dependent transmethylation. Thus, SAH is a negative feedback inhibitor of SAM-dependent transmethylation processes. As inhibition of SAH hydrolase results in the accumulation of SAH in the cell, elevated levels of SAH suppress SAM-dependent transmethylation that plays a key role in the formation of the capped methylated structure at the 5'-terminus of viral mRNA. Thus, SAH hydrolase is an attractive target for the development of broad-spectrum antiviral agents (figure 1).

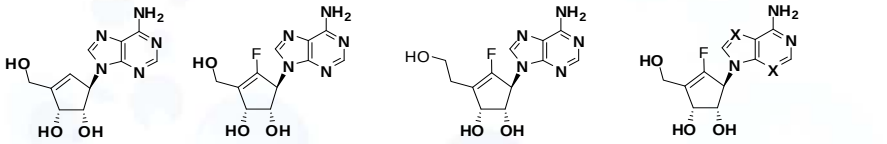

Figure 1

Neplanocin A showed potent antiviral activities against several RNA and DNA viruses but could not be further developed as a clinical agent because of high cytotoxicity due to the phosphorylation by adenosine kinase. On the basis of these observations, numerous efforts have been made to modify the structure to produce the compounds with better therapeutic efficacy. Recently, fluoroneplanocin A (**2)** was designed and synthesized as a mechanism-based inhibitor of SAH hydrolase. Fluoroneplanocin A was found to inhibit the enzyme through both type Ⅱ mechanism-based irreversible inhibition and type Ⅰ mechanism-based reversible cofactor (NAD)-depletion and it is (IC_{50}= 0.48 μM) two-fold more potent than the parent neplanocin A (IC_{50} = 0.82 μM).

Recently**, we devised a new method for the synthesis of fluorohomoneplanocin A (3) by using stereoselective epoxidation, followed by regioselective and stereoselective fluorination and finally simultaneous oxidation-elimination reaction.** Based on the same lines, we also synthesized another analogues of fluoroneplanocin A **(4)** (figure 1).

From the synthesized compound, all of the adenine derivatives exhibited potent anticancer activity in all of the human cancer cell lines.

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O-17

Attribution of Disparate Dimedone Derivatives: Synthesis as well Docking Studies against 5-HT_{2A} Receptor

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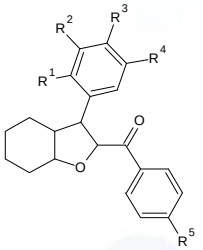
A base catalyzed sequential one-pot protocol for an effective preparation of *3-(Substitutedphenyl) -6,6-dimethyl-2-(substitutedphenylcarbonyl)-3,5,6,7-tetrahydro-1-benzofuran-4(2H)-one*derivativeshave been described. One-pot reaction of aromatic aldehydes, various Phenacylbromide and Dimedone gives corresponding substituted Benzofurans in economically affordable yields with stereo specificity at **2nd** and **3rd** position via formation of substituted Pyridiniumylides. Newly synthesized compounds were characterized by different spectral techniques such as IR, ^{1}H NMR, ^{13}C NMR and Mass spectrometry. Identification of final adduct was carried out by XRD techniques.



Furthermore,The aim of these work to develop a new 5-HT_{2A} inhibitor, that could be selective and may be a good target for drug discovery. For this target, a library was generated and docking of all this newly synthesized compounds were done using **Molecular Virtual Docking**to finding a more preferably ligands, can act a diverse 5-HT_{2A} antagonist in recent era of pharmacology.

O-18

Molecular Modeling Perspective of the Inhibitors Binding to Vinca Domain of Tubulin

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Abstract: A predictive ligand based quantative pharmacophore model has been constructed to extract essential features accountable for the inhibition of a set of vinca domain inhibitors. To generate pharmacophore model a set of 23 functionally diverse training compounds was exploited employing the PHASE algorithm. The statistically significant (R^2 = 0.81, Q^2 = 0.61, RMSE = 0.63 and Pearson-R = 0.79) five feature pharmacophore model consist of one hydrogen-bond acceptor, a hydrogen-bond donor, a hydrophobic feature, a positive ionizable and a ring aromatic feature. The model was chosen to screen the ZINC natural product database and the hits were subjected to molecular docking study using GLIDE.

The rationale behind the present work is to bid healthier perceptive about the binding of the tubulin inhibitors and abet in discovering new leads with potent antitumor activities.

Keywords: virtual screening; pharmacophore; molecular docking; antitumor; vinca

O-19

Appraisinglead-likeness descriptors for commercially available organic compounds

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A plethora of literature has been published for unveiling the issues of lead and drug like compounds. The complexity of biological system and exponentially increasing number of compounds and database seems to be challenging and needs rethinking of evaluation procedures. In this direction, we have appraise the descriptive cut-offsto assign the drug like features onto the commercially available compounds. Thereafter,evaluation of clinically available drug candidates was carried to test and train the drug like filters. This philosophy has been employed on commercially available compoundsretrieved from 10 resources andwere assessed for their potential lead like properties.Further evaluation for the physical-chemical properties and molecular diversity was also executed. The estimation of lead-likeness was performed by various descriptive filters proposed by Lipinski, Veber and Hann. Overall, a distinctive comparison is made between the druglikeness attributes of known drugs and commercial available drugs. The study provides guidelines for the selection of molecules, and allowed threshold in thumb rules to pick compounds for high throughput screening.

Keywords: drug-like filters, physical-chemical properties, high throughput screening, lead

O-20

Enzymes Mediated Synthesis and Characterization of Potent Antimicrobial Gold Nanoparticles against MDR bacteria and Development of Antimicrobial Surgical Suture

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Abstract: Due to the recent development in nanobiotechnology field, there is an ongoing demand fordeveloping the environmental friendly method for the synthesis of gold nanoparticles (AuNPs) that is pollution less and do not use the hazardous chemicals for synthesis. In the present research, we report the synthesis of AuNPs by using macerozyme as reducing agent at various temperatures scale i.e. room temperature, 60°C, 80°C and 90°C. The intensity of formation of nanoparticles was more at elevated temperature. The AuNPs were characterized by using UV-vis spectroscopy, Dynamic Light Scattering (DLS), SEM-EDAX and XRD. UV-vis indicated the surface plasmon resonance (SPR) at 520nm and DLS result suggested the average particle size was 16.06nm. The SEM-EDAX analysis confirms the detection of AuNPs by observing the characteristics peak at 2KeV on Spectrum. Furthermore, element analysis by XRD pattern at 2θ ensures the presence of Gold. To evaluate the application of AuNPs, antimicrobial activity was tested against ten pathogenic bacterial strains and five fungal pathogenic strains. Antimicrobial potency of AuNPs was also tested on clinically isolated *E.coli* ESBL+ve MDR, Oxacillin-resistant *Staphylococcus aureus* (ORSA) and *Streptococcus pneumoniae* MDR Strain. AuNPs effectiveness was very remarkable against all tested bacterial and fungal strains suggest the broad-spectrum antimicrobial nature. The antimicrobial surgical suture were also developed and tested against bacterial strains.

Keywords: Gold nanoparticles, macerozyme, MDR, Antimicrobial activity

O-21

Screening of two important alkaloids from cell suspension cultures of *Tinospora cordifolia* (Willd.) Miers ex Hook. F. & Thoms using high-throughput screening methods

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Tinospora cordifolia is one of the ancient ayurvedic medicinal plants possesses plethora of therapeutic properties. However, its natural resources are restricted. To overcome this limitation, one of the proven and potent technologies, plant tissue culture can be employed as an alternative strategy for the effective production of bioactive compounds as well as for the conservation of entire biodiversity of this plant, irrespective of regional and seasonal constraints. The establishment of cell suspension culture is one of the efficient methods for the production of bioactive metabolites where the homogenous population of highest biomass producing cell lines of *T. cordifolia* can be obtained. Therefore, the cell suspension culture was raised on Murashige and Skoog (Murashige and Skoog [1]) liquid medium supplemented with cytokinin and auxin. Further, the evaluation of biomass on the basis of fresh weight and dry weight was recorded. Moreover, the estimation of effective plant chemicals was analyzed using chromatographic and spectroscopic methods.

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O-22

Stearoyl CoA desaturase 1 (SCD1): A key target to control the development of non-alcoholic fatty liver disease (NAFLD) - study from an experimental model

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Stearoyl CoA desaturase 1 (SCD1), a microsomal enzyme, also called delta-9 desaturase (D9D), synthesizes the monounsaturated fatty acids (MUFA) from saturated fatty acids (SFA) by incorporating a double bond at 9-cis position. The ratio of SFA to MUFA plays the major role in the structural integrity and functions of biological membranes. Therefore, SCD1 is considered as the key determinant of biological functions and lipid metabolism. Dysregulation of SCD1 is reported to be associated with various metabolic diseases, such as obesity, insulin resistance, type 2 diabetes (T2D) and non-alcoholic fatty liver disease (NAFLD). Inhibition of SCD1 by synthetic compounds has been shown to improve the conditions of metabolic syndrome. In this context, here we assessed the effect of fat-soluble compound, retinol/vitamin A on the regulation of SCD1 and its impact on the development of NAFLD using high fructose diet-induced rat model. For this purpose, weanling Wistar male rats were given various experimental diets; such as control, vitamin A-deficient, high fructose and vitamin A-deficient with high fructose for a period of 16 weeks. Rats fed high fructose diet with vitamin A deficiency resulted in down-regulation of hepatic SCD1 gene expression, which also reflected in the reduction of their protein levels and its catalyzed product; MUFA levels in liver and plasma. All these data were significantly corroborated with amelioration of high fructose-induced hepatic steatosis. On the contrary, repletion of vitamin A reversed these conditions and led to over-expression of SCD1 (both at gene and protein), MUFA levels in liver and resulted in induction of hepatic steatosis. In conclusion, SCD1 is the key player in high fructose-induced hepatic steatosis and seems to be a potential therapeutic target to control/mitigate the development and/or progression of non-alcoholic fatty liver disease (NAFLD).

O-23

Design and Synthesis of Mefenamic acid Derivatives as Anti-inflammatory Agents

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Non-steroidal anti-inflammatory drugs (NSAIDs) are mainly used in the treatment of various inflammatory conditions. NSAIDs used as anti-inflammatory agents suffer from main side effects like gastrointestinal ulceration and hepatotoxicity. As a result selective COX-2 inhibitors developed to reduce the side effects associated with NSAIDs. However, selective COX-2 inhibitors suffered from major cardiovascular side effects and many of them withdrawn from the market. Thus, many new methods and strategies were developed wherein structural modifications of the existing NSAIDs were done. The main change was carried out in the free carboxylic group of the NSAIDs, which was modified to reduce side effects. In order to increase the efficacy of conventional NSAIDs with reduced side-effects various derivatives of mefenamic acid were designed. Molecular docking analysis was performed using GOLD suite and synthesis of the compounds was carried out using DCC/DMAP coupling. Molecules with a highGOLD score were screened using rat paw edema methods. From *in vivo* screening it was found that some amide derivatives of the mefenamic acid were found to be more active as compared to the parent molecule.

O-24

An efficient synthesis of some novel mannich products bearing quinoline nucleus and their microbial studies

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Abstract: In this series we have synthesis novel Mannich products 4(g-m) containing bioactive quinoline nucleus, under solvent-free condition has been developed. This method provides us high amount of yields without requiring a chromatographic separation. The structure of all new synthesis compounds was established based on elemental analysis, ^{1}H NMR, ^{13}C NMR, IR spectral data. In vitro microbial studies indicate that all are active against Gram positive (*S. aureus, Streptococcus pyogenes*), Gram negative (*P. aeruginosa* and *Escherichia coli*), *M. Tuberculosis* $H_{37}RV$ bacteria, and fungus like *Candia albicans, A. Clavatus and Aspergillus niger*.

Keywords: Solvent-free**,** Multi component reaction**,** Microbial studies**,** UV absorbing material, Mannich products

O-25

Exploratory& *in-silico* Studies, Design and Synthesis of GPR40 Modulators

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Human GPR40 receptor, also known as free fatty-acid receptor 1, is a G-protein-coupled receptor that binds long chain free fatty acids to enhance glucose-dependent insulin secretion and are therefore viable targets for diabetes and metabolic disorders. In the course of the research work, Pharmacophore generation, Molecular Docking, *in-silico* ADME studies and synthesis was performed to explore the molecular determinants responsible for the agonist action at GPR40. The generation of ligand-based pharmacophore using the standard tools within Catalyst (Accelrys) from different training sets consisted of Hydrophobic, Hydrogen Bond Acceptor and Aromatic ring features as essential aspects. For Structure based pharmacophore generation crystal structures were retrieved from protein data bank. The features were clustered and the most representative features were selected and included in the pharmacophore model which was further validated and utilized as a query tool to search 3D databases. After applying drug-like and pharmacokinetic filters to the identified hit molecules, molecular docking was carried out using SYBYL-X 1.2 among which KAG-11, 14, 15, 16 & 19 showed good docking scores compared to the reference compound Tak-875. In addition, *in-silico* ADME properties to predict pharmacokinetics at the organ level has been also studied and based on all the common features a series of the designed molecules were synthesized and analyzed. So, exploring this methodology will stimulate the design and discovery of future GPCR modulators that may prove useful in disorders associated with GPCRs signalling.

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O-26

Microwave Synthesis and Bio-evaluation of Cystine Based Bio-conjugates of Benzothiazole analogs

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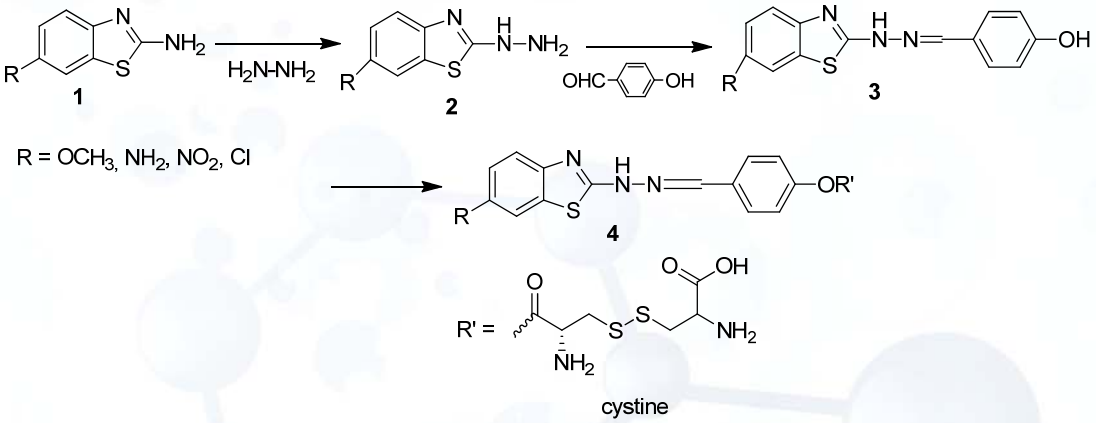
Abstract: In the current examination, somenewercystine based bio-conjugates of Schiff base were synthesized by green and clean microwave method (Scheme-1). All the synthesized compounds were in good concord with elemental and spectraldata such as^{1}H NMR,^{13}C NMR, IR and MASS spectroscopy. Physicochemical data were also recorded for all the synthesized compounds. These compounds were further screened for theirbiological activities i.e. antimicrobial and antifungal. The results supported excellent antifungal activity with MIC (minimum inhibition concentration) 6.25µg/mLin*C.albicans*. Cystine bio-conjugates were also screened for anti-cancerous potential and showed promising results with Hept- 2 cell line. The bioactivity was also authenticated with SEM study.



Scheme-1

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O-27

An effective method for the synthesis of tetra substituted Pyrazine containing nucleoside analogues

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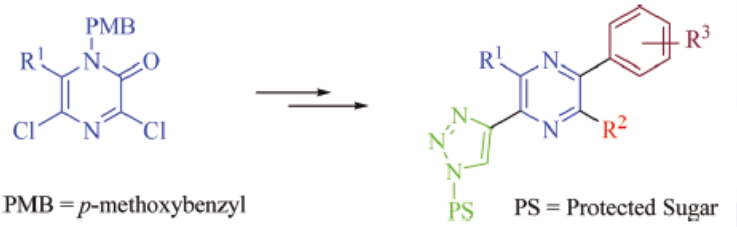
The nucleosides and their analogues have always generated considerable scientific interest in their chemistry and biology. Nucleosides are biologically active, acting as building blocks in the biosynthetic intermediates, energy donors, metabolic regulators, and cofactors in enzymatic processes. Many nucleoside analogues have been developed for screening as antiviral agents, anticancer drugs, by variation of the sugar part and/or the heterocyclic base. A substantial number of naturally occurring and synthetic nucleosides, many with interesting biological activities, have been prepared via a variety of approaches. The use of substituted pyrazines as organic bases of the nucleoside may be worthwhile to study.

An effective route for the synthesis of tetra-substituted pyrazines from pyrazin-2(1*H*)-ones have been explained. Containing pyrazine as the core, several nucleoside analogues have been synthesized via triazole linkage. The effect of microwave irradiation throughout the synthesis has also been described.



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O-28

Frankincense oil based nanoemulsified carrier system for synergistic effect and improved delivery of docetaxel

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Despite tremendous medical advancement, the havoc of cancer is still a curse for humanity at large and claims millions of lives worldwide every year. Docetaxel, a microtubule depolymerization inhibitor from plants of genus *Taxus*, is a key treatment paradigm in the treatment of various types of cancer like brain, small cell and non-small cell lung, breast, pancreatic cancer, etc. However, the intensely deleterious adverse effects of the drug and its commercial formulation Taxotere® containing ethanol and polysorbate 80 jeopardize its use in a most efficient way leading to various toxicities such as hepatotoxicity, neurotoxicity, and neutropenia, etc.. In present study, we envisioned to develop a polysorbate 80-ethanol free frankincense oil/soya oil based nanoemulsified delivery system loaded with docetaxel with an aim to acheive synergistic effect and passive targeting via enhanced permeability and retention effect. The nanoemulsion was fabricated using high pressure homogenization technique optimizing the process parameters namely operating pressure and number of cycles.The d-alpha tocopheryl polyethylene glycol 1000 succinate (TPGS) was employed to serve the dual function of the stabilizer and inhibitor of over expressed p-glycoprotein (p-gp) efflux pumps present on the tumor cell surface. The fabricated nanoemulsion was characterized suitably for size, polydispersity index, zeta potential and pH which were found to be 124nm, 0.086 and -28mV respectively. The formulation was subjected to various stressful condition like successive freeze-thaw cycles, dilution stress and high revolution stress and it successfully passed the stress test and showed good stability upto 6 months. The transmission electron microscopy studies revealed spherical shape of the droplets and were in corroboration with size obtained via Zetasizer. The release of docetaxel from nanoemulsion was sustained for 12 hours at pH 7.4.The formulation showed enhanced cellular uptake, cytotoxicity, and apoptosis in MDA-MB-231cells. The number of tumor cells arrested in G2/M phase was more and the hemolytic potential of the formulation was less than the pristine docetaxel. We hypothesized that the combination therapy of docetaxel with FO in nanoemulsified formulation will lead to an increased therapeutic efficacy with minimizing the adverse effects.

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O-29

Enantioselective Henry reaction of trifluoromethyl ketones and aldehydes using chiral copper(II)-complex and their applications

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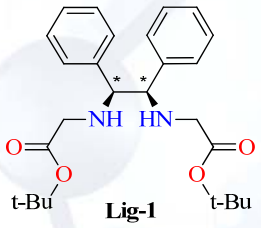
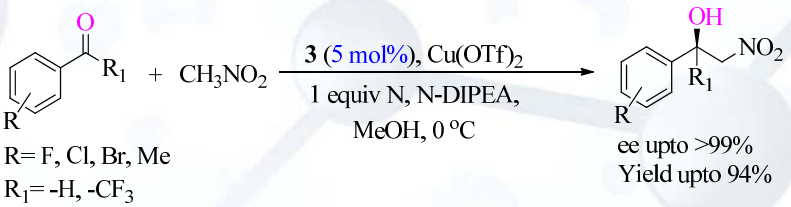
Abstract: The nitroaldol or Henry reaction is an important and atom-economic methodology for the formation of *β* -hydroxynitroalkanes providing effectual access to valuable bi-functional compounds such as 1, 2-amino alcohols and *α*-hydroxy carboxylic acids.[1] The high scientific and commercial value of enantiopurenitroaldol adduct has been testified as one of the most important building blocks for pharmaceuticals and agrochemicals.[2] During a long period of time, a huge volume of search for new, eco-friendly and effective catalytic asymmetric Henry reaction has been carried out by numerous research teams both in industry and academia.[3] Nowadays, one of the important fields of research is the organofluorinebased chemistry due to the wide range of applications of organo fluorine compounds.[4]It acts as an versatile synthon and attracted great attention in the synthetic organic chemistry.[5] Therefore, the asymmetric synthesis of α-trifluoromethyltetrasubstituted carbons having important role in many drugs like Efavirenz (anti-HIV),[6] a chiral α -trifluoromethyl tertiary alcohol in which the -CF_3 moiety is located at an asymmetric tetrasubstituted carbon centre attracted much attention. In this regard,we have synthesised a new types of chiral ligand(1R,2R)-(-)-1,2-diphenyl-1,2-diaminoethanederived from inexpensive and readily available (1*R*,2*R*)-(-)-1,2-diphenyl-1,2-diaminoethane and *tert*-butylbromoacetate. *In situ* generated complex obtained by the interaction of chiral ligand 1 with copper triflate as metal source was used for asymmetric Henry reaction of trifluoromethyl ketone having different substituents in the aromatic ring andnitromethaneas a nucleophile at 0 °C in presence of *N,N* DIPEA as an additive. Excellent enantioselectivity (*ee* upto99 %) of nitroaldol product with moderate yield (upto 80 %) was achieved in case of 2,2,2-trifluoro-1-(4-fluorophenyl)ethanone. In most of the cases, (1*R*,2*R*)-(-)-1,2-diphenyl-1,2-diaminoethane with copper triflate gave excellent enantioselectivity and yields in both electronwithdrawing and electron donating substituents.



Lig-1

(1*R*,2*R*)-(-)-1,2-diphenyl-1,2-diaminoethane,

Fig.-Energetic ligand for asymmetric Henry reaction



Scheme: Optimization reaction conditionfor asymmetric Henry reaction

Table: Variation of substrates

Entry	Substrate	Yield[b](%)	Ee[c](%)
1	2,2,2-trifluoro-1-phenylethanone	74	97
2	2,2,2-trifluoro-1-(4-fluorophenyl)ethanone	76	>99
3	2,2,2-trifluoro-1-(4-bromophenyl)ethanone	70	92
4	2,2,2-trifluoro-1-(4-chlorophenyl)ethanone	80	88
5	2,2,2-trifluoro-1-(4-methylphenyl)ethanone	62	90

[a]All the reactions were carried out with 0.5 mmol of substrate and 5 mmol of nitromethane. [b] Isolated yield after flash column chromatography. [c] Determined by HPLC.

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O-30

Inhibitory action of piperazine derivatives on mild steel corrosion in hydrochloric acid solutions

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Abstract: Derivatives of piperazine (Tert-butyl-4-(2-(ethoxycarbonyl)benzofuran-5-yl)-piperazine-1-carboxylate, Ethyl 5-(piperazin-1-yl)benzofuran-2-carboxylate and 3tert-butyl 4-(2-carbamoylbenzofuran-5-yl)piperazine-1-carboxylate) were used as corrosion inhibitors for mild steel in hydrochloric acid solution. The inhibition efficiency depended on the concentration and type of the piperazines. The inhibition efficiency ranged between 90 and 94 % at the highest concentration (25 mM), and between 44 and 62% at the lowest concentration (5 mM) of inhibitor in 1 M HCl solution. Inhibition efficiency decreased with rise in temperature, this corresponded to surface coverage of the metal by the inhibitor. Potentiodynamic polarization measurements have been carried out at room temperature, which clearly reveal the fact that all investigated inhibitors are of mixed type and they inhibit corrosion of mild steel by blocking the active sites of the metal surface. The results also showed that, the inhibitors were adsorbed on the mild steel surface according to Langmuir adsorption isotherm.

Keywords: Corrosion, Mild steel, Hydrochloric acid, piperazines, Langmuir adsorption, Temkin's adsorption isotherm.

O-31

QUINOLINE DERIVATIVES AS ANTICANCER AGENT

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In this study, a series of quinoline derivatives were synthesized and investigated their antiproliferative against various cancer cells in vitro. The result revealed that these derivatives effectively inhibited the cell growth of of a broad spectrum of cancer cell lines. Further study revealed that these derivatives may induce autophagy and result in disruption of autophagy propagation. Therefore, these derivatives activated massive apoptosis, as evidenced by PARP cleavage and caspase-9 activation. Detailed synthesis, biological activity and mechanism of action of the quinoline derivatives will be discussed in the presentation.

O-32

Zinc hexacyanidocobaltate(III) nanoparticles catalyzed oxidation of benzyl alcohol

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The catalytic activity of zinc hexacyanidocobaltate(III) nanoparticles for the oxidation of benzyl alcohol has been studied. Zinc hexacyanidocobaltate(III) nanoparticles with size rang 40-70 nm were synthesized using precipitation techniques and characterized using elemental analysis, atomic absorption spectroscopy, infrared spectroscopy, TGA/DTA/ X-ray diffraction pattern, SEM and TEM studies. The catalytic oxidation was carried out under solvent-free and heterogeneous conditions using H_2O_2 as oxidant. The oxidation product was characterized using gas chromatography. The effect of physical parameters of reaction conditions on the reaction progress has been studied and the reaction conditions such as temperature, amount of catalyst and benzyl alcohol-catalyst ratio have been optimized. The catalyst showed 30 percent conversion of benzyl alcohol under the optimized reaction conditions. The used catalyst was found to be highly selective for the oxidation product, namely, benzaldehyde. High degree of heterogeneity, high product selectivity, high stability, recyclability of catalyst and the involvement of eco-friendly oxidant (H_2O_2) indicate the green behaviour of the catalyst used herein.

Keywords: Zinc hexacyanidocobaltate(III), heterogeneous catalyst, benzyl alcohol, benzaldehyde.

O-33

Dynamics of Pluronics and their application as novel vesicular nanocarrier for drug solubilisation

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Abstract: Pluronics are the block co polymers widely used in drug delivery systems due to low toxicity and wide varieties in their molecular features. The present work focuses on the surface properties of Pluronics and the interaction with drug in the microenvironments resulted due to entropycally driven aggregation process. Different Pluronics surfactants, namely L101,L121,L81, P123,P103,P85 and P105 were studied for their equilibrium surface tension and dynamic surface tension. Three drugs with different partitioning potential were investigated for their solubilisation and consequent impact to the size and shape of the nanocarrier. The drugs used were 5-methyl salicylate, Aspirin, Exemestane with log P 2.5, 1.43 and 3.7, respectively. The formation of vesicles using triblock copolymer has been successfully characterized by optical spectroscopy and light scattering measurement. Drug induced vesicle formation was found with smaller structures like methyl salicylate and Aspirin depending on the surface properties of block copolymers.While larger structure of drug doesnot penetrate into the core region of spherical nanocarrier and thus doesnot induce vesicle formation. In order to understand the compatibility of mixed surfactant system, mixed Pluronics nanocarriers were formed for the solubilisation of such molecules. Different Pluronic nanocarrier mixed systems were formed by keeping fixed PEO content of molecules and varying the PPO portion. These nanocarrier systems can be of good potential for the drug delivery.

POSTER

P-1

Cancer treatment with Nano-Diamonds

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Abstract: Diamond nano-particles are now finding new and far-reaching applications in modern biomedical science and biotechnologies. Due to its excellent biocompatibility, nano-diamonds serve as versatile platforms that can be embedded within polymer-based microfilm devices. The nano-diamonds are complexed with a chemotherapeutic, and subsequently enable sustained/slow release of the drug for a minimum of one month, with a significant amount of drug in reserve. This opens up the potential for highly localized drug release as a complementary and potent form of treatment with systemic injection towards the reduction of continuous dosing, and as such, attenuation of the often powerful side effects of chemotherapy.

Nano-diamonds are quite economical, enabling the broad impact of these devices towards a spectrum of physiological disorders e.g. serving as a local chemotherapeutic patch, or as a pericardial device to suppress inflammation after open heart surgery. A substantial amount of drug can be loaded onto clusters of nano-diamonds, which have a high surface area. The nano-diamonds are then put between extremely thin films of parylene, resulting in a device that is minimally invasive.
Nano-diamond patch could be used to treat a localized region where residual cancer cells might remain after a tumor is removed. If a tumor has to be removed from the breast or brain, the device could be implanted in the affected area as part of the same surgery. This approach, which confines drug release to a specific location, could mitigate side effects and complications from other chemotherapy treatments.

Thus, the nano-diamonds can be used to explore a broad range of therapeutic classes, including additional small molecules, proteins, therapeutic antibodies, RNAi, etc.

Keywords: Cancer, Nano-diamond, Drug release, Nanotechnology

P-2

COMPARATIVE *IN VITRO* AND *IN VIVO* PHARMACOKINETIC EVALUATION OF NOVEL 4-AMINOQUINOLINE-TETRAZOLE ANTIMALARIALS

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Purpose: S011-0719 and S011-0725 are potent antimalarial and are active against chloroquine-sensitive (3D7) and chloroquine-resistant (K1) strains of *Plasmodium falciparum* both *in vitro* and *in vivo.*Considering the promising antimalarial activity of S011-0719 and S011-0725, *in vitro* and *in vivo* pharmacokinetic studies were performed to establish the ADME profiles in support of their development as candidate drugs.

Methods: Separate HPLC-UV methods for quantification of S011-0719 and S011-0725 in rat serum were developed and validated. To facilitate further pharmacological and pharmaceutical development,red blood cell (RBC) uptake, whole blood partitioning, serum protein binding and stability studies in simulated gastric fluid (SGF), simulated intestinal fluid (SIF) andrat liver microsomeswere performed. Single dose pharmacokinetic studies after oral (10 mg/kg) and intravenous (10 mg/kg) administration were accomplished in male *Sprague Dawley* rats. The concentration-time data were subjected to noncompartmental approach using Phoenix WinNonlin (version 6.3; CertaraInc, Missouri, USA) to determine the pharmacokinetic parameters of both the compounds.

Results: The stability studies revealed that S011-0725 was stable in both simulated gastrointestinal fluids. At the end of 2 h of incubation in SIF, S011-0719 showed 54% degradation but was found stable in SGF. Microsomal stability studies demonstrated that both the compounds were metabolized by phase I enzymes. At the end of 1 h of incubation in rat liver microsomes, 58.6 and 35.5% of S011-0719 and S011-0725, respectively, remained unchanged. The oral and intravenous pharmacokinetic study of S011-0719 and S011-0725 in the male *Sprague Dawley* rats revealed that the compounds were quickly absorbed, distributed and slowly eliminated from the serum with an elimination half-life of 5.3 and 22.6 h, respectively.

Conclusions: S011-0725 is more appropriate for oral therapy than S011-0719 due to its stability in SIF; 14-times lower clearance, 1.9-times higher AUC and 3.3-times higher MRT after a single oral dose of 10 mg/kg.

P-3

COMPARATIVE LOGARITHMIC PARTITION COEFFICIENT STUDY OF SYNTHESIZED FIVE MEMBERED LACTAM DERIVATIVES FOR LIPOPHILICITY

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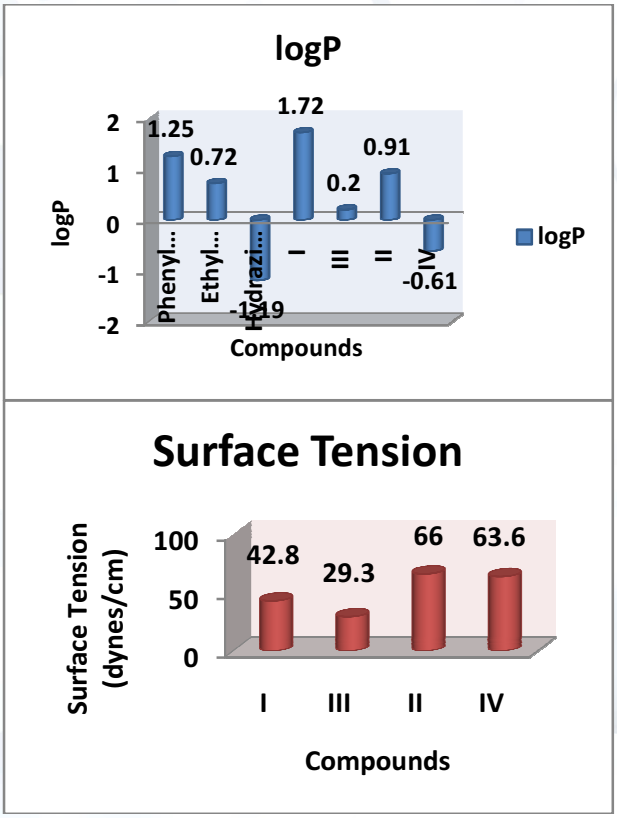
Abstract: Five membered heterocyclic moiety (pyrazolone) has been synthesized by reacting between phenyl hydrazine and hydrazine with β-keto ester (ethyl acetoacetate) by condensation reaction to get the desired moiety which on alkaline permanganate oxidation gives the corresponding carboxylic acid derivatives in two series. The four compounds (I & II) of 1st series and (II & IV) of 2nd series were characterized for structural framework. The **logP** profile of all four compounds is as follows:

Reagents: [Highest] Phenyl hydrazine > Ethyl acetoacetate > Hydrazine hydrate [Lowest]

Compounds: [Highest] I (5-methyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one) > II (5-oxo-1-phenyl-2,5-dihydro-1H-pyrazole-3-carboxylic acid) > III (5-methyl-1,2-dihydro-3H-pyrazol-3-one) > IV (5-oxo-2,5-dihydro-1H-pyrazole-3-carboxylic acid) > [Lowest]

This logarithm of partition coefficient of all the said items is totally dependent on the polarity and solubility of the matters. The hydrophobicity and hydrophilicity of all synthesized four compounds depend on logP values due to the substituted functional groups of pyrazolone ring. Phenyl/Methyl/Carboxylic acid the three main chromophore groups change their logP parameters as well as surface tension.



logP profile:

I (5-methyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one)>II (5-oxo-1-phenyl-2,5-dihydro-1H-pyrazole-3-carboxylic acid)

III (5-methyl-1,2-dihydro-3H-pyrazol-3-one)>IV (5-oxo-2,5-dihydro-1H-pyrazole-3-carboxylic acid)
Surface tension profile:

I (5-methyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one)<II (5-oxo-1-phenyl-2,5-dihydro-1H-pyrazole-3-carboxylic acid)

III (5-methyl-1,2-dihydro-3H-pyrazol-3-one)<IV (5-oxo-2,5-dihydro-1H-pyrazole-3-carboxylic acid)
Lipophilicity and hydrophilicity of all compounds depend on the substitutions. Phenyl group is more lipophilic than methyl and carboxylic acid group is more hydrophilic so IV becomes liquid but II becomes solid due to the presence of phenyl ring but I is more lipophilic than III due to the presence of phenyl ring in I and III is more hydrophilic due to the presence of methyl group. Main ring pyrazolone is common in all I-IV: I (phenyl+methyl), II (phenyl+carboxylic acid), III (methyl), IV (carboxylic acid). I & III produce white compounds and II & IV are orange compounds in which IV is found liquid and rest all are solids which have been characterized by UV spectra and obeys wavelength of UV & Visible spectra.

Keywords: Pyrazolone, Pyrazolone carboxylic acid, logP, $KMnO_4$/KOH oxidation, H_2O_2 oxidation, Polarity, Partition coefficient, Surface tension

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P-4

Structural polymorphism exhibited by a quasipalindrome present in Human *SCAI* gene

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Structural polymorphism isconsidered themost prevalent characteristic of DNA. In order to understand this perception more clearly, a single nucleotide polymorphism (SNP) siteof human *SCAI* gene was studied where a T→Gbase change in a quasipalindromicsequencedemonstrates structural difference between the two alleles.We present here some results of our study on a 24-mer DNA sequence [SG24T; ACGTCGACGTGGG(T/G)ACGTCGACGT], which lies in the intronic region of*SCAI* (suppressor of Cancer Cell Invasion) gene. *SCAI* is a highly conserved protein that regulates invasion cell migration. Report reveal that decreased levels of *SCAI* are tightly correlated with increased invasive cell migration i.e., it is downregulated in several human tumours(1).Further, *SCAI* inhibits the MAL/SRF transcriptional activator complexresulting into the reduced expression of beta1-integrins and decrease in the invasive potential (2). With the help of biophysical techniques : Circular Dichroism spectroscopy, UV-Thermal melting studies and Gel Electrophoresis, we demonstrated that SG24T forms a hairpin structure whereas with T→G SNP change,i.e, the SG24 sequence exhibited a hairpin-duplex equilibrium at physiological pH and salt condition. It strongly suggests the possibility of structural transition between hairpin andduplex at quasipalindromic region. The structural variation may be considered as a new pathway in molecular recognition and drug development.

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P-5

A Convenient Synthesis of Biologically Important Thiazoline Scaffolds

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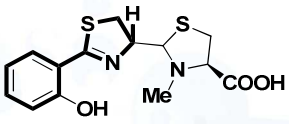
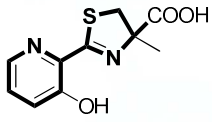
Thiazolines are significant structural motifs that are found in natural products and numerous biologically active molecules which show therapeutic activities such as anti-HIV, antimicrobial, anticancer, antibiotic, antitumour, etc. The general approach for the synthesis of thiazolines involves the condensation of aminothiol with different precursors such as carboxylic acids, esters, nitriles, aldehydes, iminoethers, etc [1]. However, most of these transformations require the use of a variety of catalysts, harsh reaction conditions, longer reaction hours with high temperatures, etc. As part of our research work on the convenient synthesis of biologically important molecules, we have recently reported the regioselective synthesis of novel *N*-(hydroxyalkyl)cinnamamides mediated by Na_2CO_3 [2]. Also, very recently, we have reported metal- and catalyst-free synthesis of 2-aryl/heteroaryloxazolines which involves the reaction of aromatic nitrile with aminoalcohols in the presence of Na_2CO_3 as base [3]. Presently, we are involved in developing a convenient protocol for the synthesis of biologically important thiazoline scaffolds. This work will be discussed in greater details during the poster presentation.



Pyochelin



Desferrithiocin
(iron chelator)

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P-6

To explore the structural difference between the ε3 and ε4 allele SNP of the human apolipoprotein (*APOE*) gene

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Alzheimer's disease is a neurological disorder that has been considered as the most common cause of dementia which results into loss of memory and intellectual abilities among adults aged 65 or above. According to early reports, apolipoprotein E (*APOE*) gene has been associated with Alzheimer's disease [1]. It helps in maintaining normal cholesterol levels by combining with lipids to form lipoproteins that remove excess cholesterol from the blood. Three different isoforms of *APOE* gene ε2, ε3 and ε4 are well studied and it is reported that ε4 allele of *APOE* gene increases the risk of developing late-onset Alzheimer's disease whereas ε3 is the most common among the general population [2]. The *APOE* ε4 allele is defined by SNP rs429358 which differs from the common ε3 type by only one nucleotide base change at position +2985 from TSS. These changes can immensely alter the structure and function of *APOE* gene [3,4]. In the present study, we have selected a 22-mer DNA sequence (APOE22T) found in exon 4 of the APOE gene and its SNP (APOE22C) depicting a single base change from T→C to study the structural differences between the two alleles. With the help of biophysical techniques like Circular Dichroism spectroscopy, UV-Thermal melting studies and Gel Electrophoresis, we demonstrated that APOE22T reflecting the ε3 version forms a hairpin structure whereas with T→C SNP change, the APOE22C sequence exists as an antiparallel duplex at physiological pH and salt condition. This structural change may be responsible for alteration of APOE structure and function that further increases the risk of developing Alzheimer's disease.

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P-7

Visible light-Assisted selective oxidation of C_{sp3}-H of methyl arenes into carbonyl compounds

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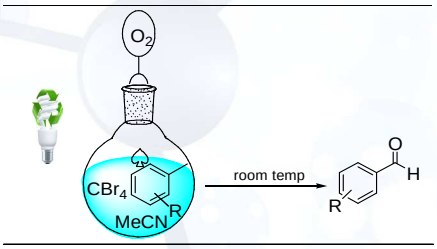
The fundamental objective for chemists is to develop new sustainable routes for chemical transformations having significant concept and practical interest under placid reaction conditions. In this context, visible light mediated photoredox catalysis has emerged as a state-of-the-art alternative to advance this goal [1], especially because of its eco-compatibility, easy availability, safe handling and everlasting abundance as an energy source. Also, several synthetic protocols are known applying visible light photoredox catalysis in conjuction with highly expensive and potentially toxic ruthenium and iridium complexes as photosensitizers, therefore, the development of metal-free photocatalytic route for chemical transformations are warmly welcomed especially in terms of economical and environmental issues.

Also, among various methods, oxidation reactions having unique advantage to activate the inert bonds, especially C-H bonds, play a pivotal role in the chemical industry for designing the chemical intermediates and fine chemical specialties [2]. However, selectivity of oxidation is still an open challenge for chemists. Cumulatively, carbonyl compounds, the vital substrates in organic synthesis, are still synthesized by non- eco-compatible methods with very low atom economy involving copious amount of waste generation. Hence, selective oxidation of methylarenes into synthetically important carbonyl compounds is quite demanding concerning both reactivity and selectivity issues.

Encompassing aforementioned facts, we hypothesized visible-light-mediated one-pot selective oxidation of methyl arenes employing CBr_4 as a lenient and efficient photoredox catalyst and molecular oxygen as an oxidant (Scheme 1). With this perspective and valuable facts herein we disclose the metal-free, visible light mediated efficient route for the selective oxidation of methyl arenes up to aromatic aldehydes only.



Scheme 1 Selective oxidation of methyl arenes into aromatic aldehyde

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P-8

Carbon tetrabromide mediated synthesis of 2-aminothiazoles via oxidative cyclocondensation of ketones and thioureas

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Aminothiazole heterocycles have been explored as building blocks in organic synthesis and material science [1]. They are also a privileged structural motif in numerous biologically active molecules [2]. Aminothiazoles are also known to be ligands of estrogen receptors as well as of adenosine receptor antagonists [3]. Analogs of aminothiazole have also agricultural importance for being used as fungicides [4]. There are various methods reported for the synthesis of 2-aminothiazoles, but recently, Wang and coworkers obtained 2-aminothiazoles by KI/NH_4NO_3 catalyzed aerobic oxidative cyclization of ketones and thioureas in ionic liquid [5]. The method requires several catalysts/reagents which makes this protocol less economical and convinient. Carbon tetrabromide is a commercially available and cheap reagent, which has found various applications in organic transformations [6]. Our protocol involves the formation of sulfenyl bromide as an umpolung intermediate of nucleophilic sulfur, which is responsible for C-S bond formation leading to oxidative cyclization of ketones and thioureas to furnish the desired products. Carbon tetrabromide was used as a convenient and mild brominating reagent under basic condition at room temperature to give 2-aminothiazoles in good to excellent yields. The method is metal-free, highly efficient and works in operationally simple manner at room temperature. Thus, it offers a superior alternative to the existing methods for the synthesis of 2-aminothiazoles.

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P-9

Design and Synthesis of Some Novel Hybrid Heteroannulated Pyrimidine Derivatives for Their Biological Activity

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Pyrimidine moiety plays significant role in medicinal chemistry because it is an important constituent of nucleic acid, moreover, these pyrimidines derivatives are fond to have a wide range of pharmacological applications [1-5] as anticancer, diuretics, antihypertensive, analgesic, antihistaminic, antimalerial, antileishmanial, antiviral, antifungal, and antibacterial drugs. . In our continuous effort to synthesize heterocycles for biological significance [6] and keeping in view importance of pyrimidines in antiparasitic area, recently, we have synthesized some novel pyridine and heteroannulated pyrimidine based hybrid derivatives for their biological activity. In this presentation, the details synthetic procedure, plausible mechanism and characterizations of the synthesized compounds by the various spectral data (FTIR, UV, ^{1}H NMR, ^{13}C NMR and EIMS) analysis will be discussed.

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P-10

Zinc oxide catalyzed simple and clean method for the synthesis of tertiary amines in aqueous medium

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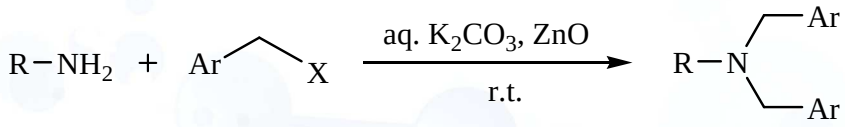
Abstract: Amines are wide spread naturally occurring biologically active compounds used in the chemical industry as basic intermediates to prepare fine chemicals, pharmaceuticals, and agrochemicals, Seayad et al [1].They display an important role in chemotherapeutic approaches to a variety of diseases, Bergeron et al [2]. The straightforward route leading to the synthesis of tertiary amines is the direct alkylation of secondary amines with alkyl halides, Salvatore et al [3]. The significant achievements in the copper and palladium catalyzed arylation of amines have been limited due to requirement of anhydrous conditions, air sensitivity, high cost and toxicity, Kuwano et al [4]. Recently, Varma et al., reported the microwave irradiation method for the direct formation of unfunctionalized tertiary amines [5]. Even though this method is relatively environmentally friendly, requires the use of specialized microwave equipment and not useful for the synthesis of these compounds on large scale. Consequently there is a need to develop synthetic methods which will avoid the use of expensive reagents and organic solvents.



Scheme 1

Zinc oxide (ZnO) is an inexpensive and commercially available inorganic solid has been used as catalyst in number of chemical transformations. Herein, we report a new, simple and environmentally benign zinc oxide catalyzed N-alkylation of primary amines by alkyl halides for the synthesis of tertiary amines in aqueous medium (Scheme 1).

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P-11

BINDING INTERACTION OF DNA WITH VARIOUS DRUGS

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Abstract: DNA plays key physiological roles in the life process. Small molecules can bind to DNA via covalent or non-covalent interactions, resulting in alteration or inhibition of DNA function. Therefore, the investigation on the binding interaction of DNA with small molecules is helpful to understand the structural features of DNA, origin of some diseases and action mechanism of some drugs, and also assists in designing improved drugs that target cellular DNA. The specific binding of drug with DNA could induce a change in conformation and also thermodynamic stability in DNA.

In the present work the binding interaction of fumaric acid, sulfosulfuran, and napthylamine with DNA was studied using UV–vis absorption spectroscopy technique [1]. The experimental results revealed that there was obvious binding interaction as there was no hyperchromism and hypochromism effect. Fumaric acid is a key intermediate in the tricarboxylic acid cycle for organic acid biosynthesis in humans and other mammals. Sulfosulfuron is an effective herbicide in nursery production and landscapes because of its effectiveness in controlling sedges. There is sufficient evidence in humans for the carcinogenicity of naphthylamine.

The activity of these molecules with salivary amylase was also studied and results were compared with activity of activator i.e. NaCl. Fumaric acid and Sulfosulfuran are more effective than activator in increasing the activity of salivary amylase. These revelations would open up possibilities for future development in food science, food chemistry, biomedicine and clinical medicine.

References:

1. Jie-Hua Shi, Jun Chen, Jing Wang, Ying-Yao Zhu, College of Pharmaceutical Science, Zhejiang University of Technology, Hangzhou 310032, China

P-12

MINERAL ION COMPOSITION OF SOME SALT TOLERANT PLANTS WITH MEDICINAL IMPORTANCE GROWING NEAR KANDLA PORT IN KACHCHH REGION

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Abstract: Salinity including secondary salinization, has been posing a tough challenge to the mankind, especially to the inhabitants of the arid and semi-arid regions of the world. Salt affected soils lose their productivity and possibility of turning such soils into productive ones, involves chemical, physical and biological reclamation. The present investigation was undertaken to examine various mineral ions present in these plants which can help in understandingthe important medicinal properties of salt tolerance plants and it may also help for understanding mechanism in halophytic plants. Leaves of the *Salvadorapersica*, *Suaedafruticosaand Salicornia brachiate*plants and soil samples were collected from the marshy habitats near the Kandla Port trust near Gandhidham.

Keywords: mineral ion, medicinal importance, salt tolerant, Kachchh

Soil characteristics
Physico-chemical

Parameter	**Result**
pH	8.3
Salinity	30.5 dS m^{-1}
Na^{+}, meq.g^{-100}	29.96
Cl^{-}, meq.g^{-100}	33.75
Ca^{2+}, meq.g^{-100}	1.54
Mg^{2+}, meq.g^{-100}	3.38
K^{+}, meq.g^{-100}	0.5

Mineral ions

Na+	29.96
Cl-	33.75
Ca2+	1.54
Mg2+	3.38
K+	0.5 meq

Heavy metals

	Succulent		**Non-succulent**	
	S. brachiata	***S. nudiflora***	***S. persica***	
Zinc	39 ug/g			
Manganese	324			
Copper	18			
Lead	9			

Heavy metal	Concentrations (µg/g)
Zinc	39
Manganese	124
Copper	18
Lead	9
Cadmium	Trace
Chromium	Trace

Plants
Physico-chemical

	Succulent		Non-succulent	
	S. brachiata	***S. nudiflora***	***S. persica***	
pH			7.8 – 8.5	
			10.5	

Mineral ions

	Succulent		Non-succulent
	S. brachiata	***S. fruticosa***	***S. persica***
Na^+, meq.g^{-1}d.wt.	3.95	2.14	1.09
Cl^-, meq.g^{-1}d.wt.	5.32	3.56	2.13
Ca^{2+}, meq.g^{-1}d.wt.	0.23	0.78	1.64
Mg^{2+}, meq.g^{-1}d.wt.	1.04	0.56	0.96
K^+, meq.g^{-1}d.wt.	0.23	0.31	0.49

Amino acids	Succulent		Non-succulent
	S. brachiata	***S. fruticosa***	***S. persica***
Alanine	√	√	√
Aspargine		√	√
Aspartic acid	√	√	√
Glutamine	√	√	√
Glycine	√	√	√
Isoleucine	√	√	√
Leucine	√	√	√
Methionine	√	√	√
Phynylalanine		√	√
Proline	√	√	√
Serine	√	√	√
Threonine	√	√	√
Tyrosine			√
Valine	√	√	√
r-amino butyric acid	√		√

P-13

SYNTHESIS AND CHARACTERIZATION OF SOME NOVEL 2-AMINO-*N*-[4-(MORPHOLIN-4-YL) PHENYL]BENZENESULFONAMIDE AND THEIR DERIVATIVES.

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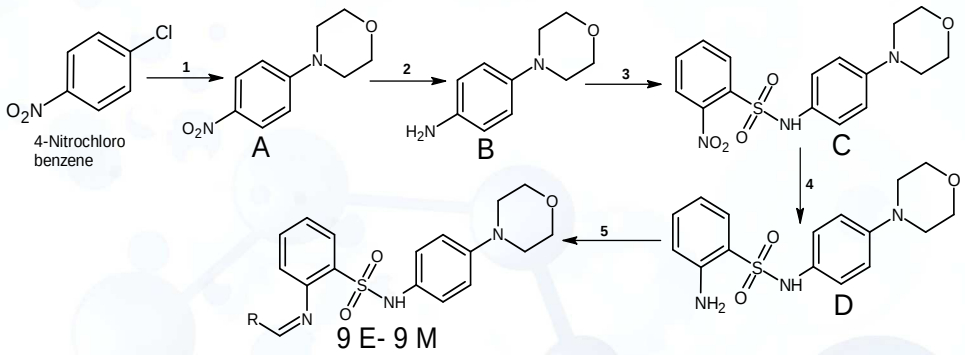
Abstract: A new effective approach to the synthesis of novel Schiff base compounds (9 E – 9 M) of 2-amino-*N*-[4-(morpholin-4-yl) phenyl]benzenesulfonamide have been synthesized from commercially available 1-Chloro-4-nitrobenzene as a starting material. The reaction conducted with help of microwave irradiated organic synthesis. The Schiff base formation reaction consumes 12-18 hour in normal conventional heating methods, but using microwave irradiation the reaction was more fast and dramatically reducing the time 4–6 min. The chemical structures of the synthesized compounds were confirmed by means of ^{1}HNMR and mass spectral data. Also were the synthesized compounds were going to be examining their antibacterial and antifungal activities in future.



Reaction Conditions: 1) $CHCl_3$, Morpholine, TEA, Reflux 16hr, 96%; 2) MeOH, 10% Pd-C, H_2, rt 5hr, 98%; 3) DCM, TEA, 2-Nitrobenzenesulphonyl chloride, 0°C 1hr, 91%; 4) DCM, DMF, 10% Pd-C, H_2, rt 5hr, 96%; 5) EtOH, Corresponding aldehydes, Microwave 65°C 4-6 min, 86-96%.

Keywords: Benzenesulfonamide, Schiff base, Morpholine, Microwave.

P-14

Total synthesis and structural reassignment of diosniponol A & B

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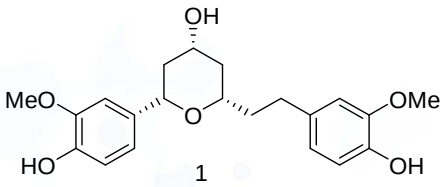
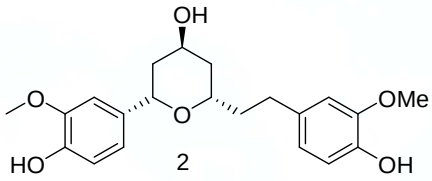
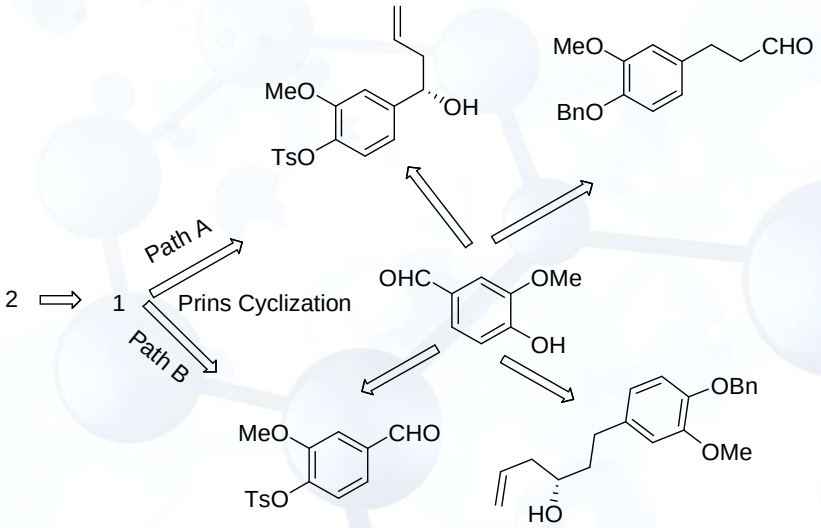
Kang Ro Lee and coworker[1] isolated two new cyclic diaryl heptanoids (having tetrahedron core) from rhizomes of *Dipponica* and named them Diosniponol A and B along with some known comounds. The compounds with diaryl motif are ubiquitous and attract significant attention due to their important biological activities like antifungal, [2] antioxidative,[3]anticancer[4] and antidepresent.[5] Diaryl heptanoids and their derivatives exhibit mainly anti neuroinflammatory and and anti inflammatory properties. The absolute structure was assigned based by 2D NMR studies with earlier known compound.







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P-15

Synthesis and Characterization of carbazole based aniline copolymers via Electrochemical approach

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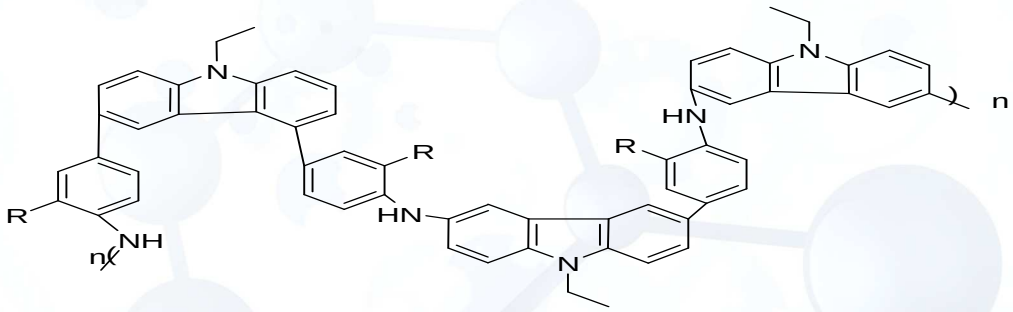
Electrochemical copolymerization of carbazole and substituted aniline monomer were studied at platinum electrode in acetonitrile solvent with Tetra butyl ammonium perchlorate (TBAP) and boron trifluoride diethyl etherate (BFEE) as supporting electrolyte via constant potential electrolysis (CPE). The polymers containing carbazole moieties have been widely studied as an important functional material for organic electronics, such as organic lighting emitting diodes (OLED), photovoltaic cells, electro chromic display, electroluminescent devices, transistors and sensors, because of their excellent hole-transportation and photoconductivity [1-3]. Electrochemical polymerization has been proved to be one of the most useful approaches for conducting polymers synthesis with several advantages. It can form conducting thin film on the working electrode by one step, the amount of polymer deposited on the electrode can be controlled by the integrated charge passed through the cell [4-6]. The present work led to the progress of a facile and environmentally benign strategy with high atom economy and excellent purity by the use of BFEE as supporting electrolyte. The copolymerization was studied by a cyclic voltammeter and the products were characterized by UV-Visible, FTIR, ^{1}H-NMR, SEM and elemental analysis.



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P-16

Synthesis and biological evaluation of azetidinone derivatives as antibacterial and antifungal agents.

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Abstract: We have developed a novel approach for the preparation of *N*-[(*Z*)-arylmethylidene]pyrrolidine-2-carboxamideusing catalytic acetic acid through the reaction of different substituted benzaldehyde with prolinamide. These molecules were further cyclized with chloroacetylchloride under nucleophilic substitution reaction condition to finally afford 3-chloro-4-aryl-1-[(2*S*)-pyrrolidin-2-ylcarbonyl]azetidin-2-one[1,2,3].These synthesized compounds were further confirmed by IR, ^{1}H NMR, and mass spectroscopy. All these final synthesized compounds are being planned to be screened for their biological activity against different strains for their antibacterial and antifungal activity.

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P-17

Synthesis and characterization of (R)-3-(4,6-dimethoxy pyrimidin-2-yl)-2-substituted thiazoldin-4-onesas antimicrobial & antifungal agents

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Abstract: Thiazolidinone is considered as a biologically important active scaffold that possesses almost all types of biological activities[1-5].(R)-3-(4,6-dimethoxy pyrimidin-2-yl)-2- substituted thiazoldin-4-oneswere prepared from (Z)-*N*- substituted benzylidine-4,6-dimethoxypyrimidin-2-amines using thioglycolic acid in the presence of anhydrous $ZnCl_2$. (Z)-N-substitutedbenzylidine-4,6-dimethoxypyrimidin-2-amineswere prepared by the reaction of 2-amino-4,6-dimethoxy pyrimidine with various aromatic aldehydes. The reactions were monitored by TLC. Some representative compounds were characterized by IR , ^{1}H , ^{13}C NMR. Newly synthesized compoundswere evaluated for their antimicrobial activity against several Gram positive and Gram negative bacteria and some selected fungal species.

Keywords: Thiazolidinone, antimicrobial activity, ^{13}C NMR, Benzylidines

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P-18

A simple and efficient procedure for the Knoevenagel condensation catalyzed by [MeHMTA]BF_4 ionic liquid

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Abstract: Ionic liquids have emerged as environmentally benign solvents and catalysts for many important organic reactions.[1] The Knoevenagel condensation reaction is a useful reaction in organic synthesis that has been employed for carbon–carbon bond formation. It is usually performed in organic solvents in presence of common bases such as ammonia, primary or secondary amines and their salts.[2] Hexamethylenetetramine-based ionic liquid, 1-methylhexamethylenetetraminium tetrafluoroborate, has been used as a catalyst for a simple and efficient method for Knoevenagel condensation of active methylene compounds and various carbonyl compounds affording products of very high yields within short duration. This method is very simple, clean and avoids hazardous organic solvents. Most of the products required no further purification. In this process, after stirring for a few minutes, the product is isolated in pure form for both solid and liquid products. The catalyst is easily recovered and can be recycled.

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P-19

Control Release of Hyaluronic Acid using Optimized Implantation Technology in Contact Lens

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Abstract: Hyaluronic acid (HA) is widely used to treat signs and symptoms of dry eye syndrome. It is commonly delivered via eye drops, which is highly inefficient due to a low bioavailability. Contact lenses are widely used for sustained drug delivery, but incorporation of drug or formulation in contact lens material, affects the optical and physical property of lenses. In present study we have designed a novel HA-laden ring implant in contact lens, to bypass any alterations in critical property of contact lens material. The objective was to provide sustained ocular delivery of HA using ring implanted hydrogel contact lenses, which can increase ocular residence time of HA. Optimization of HA-implant was carried out using 32 factorial design, by tailoring amount of cross linker and thickness of implant to achieve sustained HA release with constraint on Na+ ion permeability. In-vitro flux study results showed sustained release up to 9 days, by fabricating implant with 78.4 µm thickness and using 0.925 % of cross linker, with Na+ ion permeability > 1.5 × 10-6 mm2/min. Cytotoxicity and animal study demonstrate the safety of implant hydrogel contact lenses. In-vivo pharmacokinetic study in rabbit tear fluid showed significant increase in mean residence time (MRT) and area under curve (AUC),with HA-implant contact lenses in comparison to eye drop therapy. The study demonstrated the promising potential of implantation technology to deliver hyaluronic acid without compromising optical and physical properties of contact lens.

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P-20

Osteogenic potentials of Constituents of *Dalbergia sissoo* Roxb. Leaves

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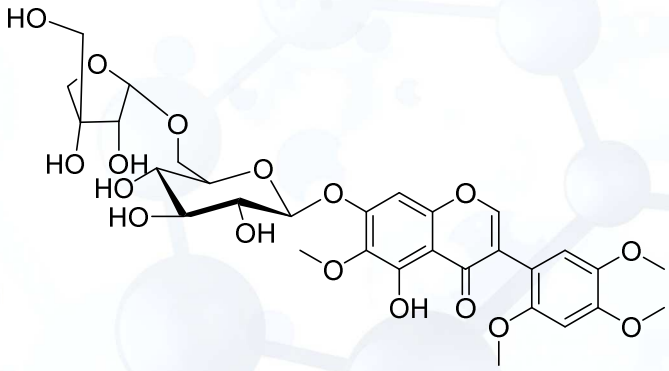
Dalbergia sissoo Roxb. belongs to the legume family (Fabaceae), is a large deciduous perennial tree, growing widely in lowland region throughout India, Pakistan, Bangladesh, Afghanistan and Nepal. *D. sissoo*, popularly known as 'Indian rose wood' and 'Shesham' has been used as traditional medicine for the treatment of gonorrhoea.[1]From previous phytochemical studies, *D. sissoo* leaves showed antipyretic, analgesic and antimicrobial properties[2] and known for the treatment of inflammation[3] and diabetes.[4] We isolated one new isoflavone glucoside, caviunin 7-O-[b-D-apiofuranosyl-(1→6)-b-D-glucopyranoside] (**1**) and a new itaconic derivative, (E)-4-methoxy-2-(3,4-dihydroxybenzylidene)-4-oxobutanoic acid (**2**) along with series of isoflavones and flavonols with their glucosides and a lignan glucoside were isolated from the ethanolic extract of *D. sissoo* leaves. The structures of these compounds were established on the basis of IR, UV, ^{1}H and ^{13}C NMR, DEPT, COSY, HSQC, HMBC and MS data. All compounds were assessed for osteogenic activity in primary calvarial osteoblast cultures. New compounds **1** and its analogue increased alkaline phosphatase activity and mineralization thus resulting in significant osteogenic activity.[5]



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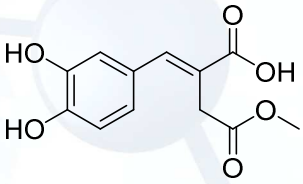

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P-21

An expeditious green synthesis of biologically active (*E*)-3-bromo-4-(substituted-phenyl)-1-(3-(pyridin-4-yl)-5-(3-(trifluoromethyl)styryl)-4*H*-1,2,4-triazol-4-yl)azetidin-2-ones

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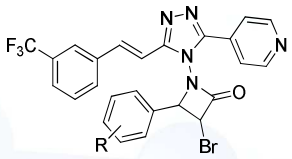
Abstract: β-Lactam posture of azetidin-2-one has been recognized as an important pharmacophore for the synthesis of a large number of entities having different biological significance[1]. With this concern number of methods have been developed to synthesize β-lactam segment via conventional[2] as well as non-conventional approach[3-5]. The present work narrates an expeditious synthesis of azetidin-2-ones by microwave as it provide simplicity in operation, intensified yields, lower energy usage and greater selectivity with less consumption of time. (*E*)-*N*-(substituted-benzylidene)-3-(pyridin-4-yl)-5-((*E*)-3-(trifluoromethyl)styryl)-4*H*-1,2,4-triazol-4-amines **3a-j** were cyclized using bromoacetylbromide to offered titled compounds **4a-j** under microwave irradiation beside with conventional method. All the synthesized compounds were characterized by spectral analysis (IR, NMR and Mass) and were screened for antimicrobial activity that compared with the standard drugs.



Keywords: Microwave, isonicotinic acid, azetidin-2-one, 1,2,4-triazole, antimicrobial

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P-22

Synthesis and antimicrobial evaluation of 4-methyl-3-nitro-2-oxo-2*H*-Chroman-7yl-2-(4-(4-fluorophenyl)-6-phenyl-2*H*-1,3-oxazin-2-yl amino)acetates

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Abstract: Coumarin segment demonstrates remarkable broad spectrum of different biological activities with that oxazine derivative enhance the pharmacological profile. In view that we have synthesized some newer oxazines based on coumarin, screened for their antimicrobial studies. 4-(4-Fluorophenyl)-6-phenyl-2*H*-1,3-oxazin-2-amines(**IIa-j**) condensed with 4-methyl-3-nitro-2-oxo-2*H*-chromen-7-yl chloroacetate(**I**) to afford 4-methyl-3-nitro-2-oxo-2*H*-chroman-7yl-2-(4-(4-florouphenyl)-6-phenyl-2*H*-1,3-oxazin-2-yl-amino)acetates(**Va-j**). The newly synthesized compounds were established by IR, NMR and mass spectral studies and were screened for their antimicrobial activities which were compared with standard drugs.

Keywords: Coumarine, oxazine, chalcone, urea

P-23

Synthesis and Characterization of Copper(II) based potential photosensitizers: Evaluation of their DNA binding profile and photo-induced DNA cleavage activity

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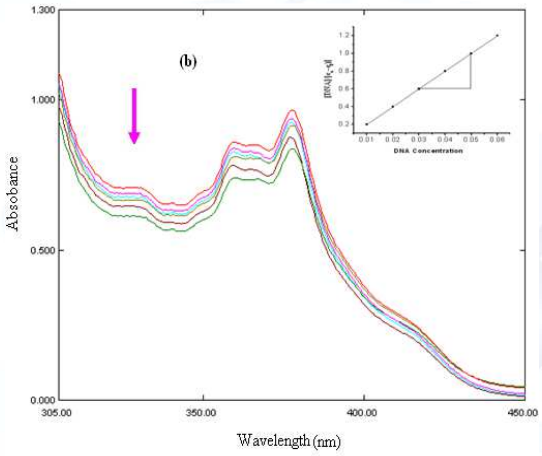
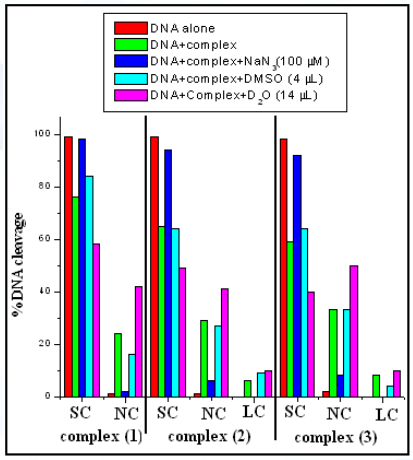
Complexes of formulation $[Cu(mqt)(B)H_2O]ClO_4$(**1-3**) of 2-thiol 4-methylquinoline and phenanthroline bases (B), viz 1,10-Phenanthroline (phen in **1**), Dipyrido[3,2-*d*:2',3'-*f*]quinoxaline (dpq in **2**) and Dipyrido[3,2-*a*:2′,3′-*c*]phenazine (dppz in **3**) have been prepared and structurally characterized by elemental analysis, IR, UV–Vis, magnetic moment values, EPR spectra and conductivity measurements. The spectral data reveal that all the complexes exhibit square-pyramidal geometry[1]. The mode of binding interactions of synthesized complexes with CT–DNA was monitored by absorption spectral titrations, viscosity measurements and thermal denaturation studies. The DNA binding constants for complexes **(1)**, **(2)** and **(3)** were determined to 2.2 $x10^3$, 1.3 x 10^4 and 8.6 $x10^4$ M^{-1} respectively. The experimental results suggest that these complexes interact with DNA through groove-binding mode[2-3]. The photo-induced cleavage reactions of the Cu(II) complexes with plasmid DNA (pUC 19) was studied using agarose gel electrophoresis technique. The photonuclease experiments demonstrated that Cu(II) complexes could act as effective DNA cleaving agents under physiological conditions. Noticeably, these three complexes have been found to be efficient photosensitizers for strand scissions in pUC19 DNA.[4-5]

Keywords: binding interactions; photosensitizers; binding constants; photonuclease activity.



DNA binding studies of Cu(II)complexes



Cleavage of SC pUC19 DNA by Cu(II) complexes

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P-24

2-(Substituted piperazine)-*N*-{4-(4-chlorophenyl)-6-[4-(dimethylamino)phenyl] pyrimidin-2-yl}acetamideds: Synthesis and their antimicrobial studies

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Abstract: Piperazines[1,2] mainly showed pharmacologically activity like anthelmintic, anticancer & antidepressant but some of its derivatives[3] also active against bacteria. The present work focused on the synthesis, antimicrobial & antituberculosis activity of piperazine containing pyrimidine moiety. 2-Chloro–*N*-{4-(4-chlorophenyl)-6-[4-{dimethylamino)phenyl]pyrimidin-2-yl}acetamide were allowed to react separately with different piperazines in presence of alkaline medium to yield the corresponding substituted heterocycles ($H_{1\text{-}9}$). The compounds obtained were identified by spectral data (IR & NMR) and screened for antimicrobial [4] and anti tuberculosis activity. The result showd that most of samples are moderately active against various micro organisms where as compound H_1, H_7, H_8 showed anti tuberculosis activity.

Keywords: Pyrimidin, piperazine, antimicrobial

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P-25

GC-MS based multivariate analysis of medicinal mushrooms

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Several kinds of mushrooms bearing beneficial properties are known to thrive in India, of which *Cordyceps sinensis* (CS) and *Ganoderma lucidum* (GL) are prominent in exhibiting antioxidant, immune-enhancing, anti- inflammatory, etc. effects. CS grows on caterpillar insect hence it is also named as 'winter worm summer grass' Pal et al. [1, 2]. GL is referred to as Reishi or 'God's Herb' and has been widely used for over 2000 years in China owing to its healing effects Bhardwaj et al [3]. In this paper, we report a GC-MS based comparative analysis of different extracts and fractions of CS and GL for the identification of volatile organic compounds.

The study reported here involves raw CS as a whole body for its aqueous extract which was obtained using accelerated solvent extraction (ASE). ASE was also employed to prepare GL mycelium and fruiting body extracts, sequentially using water, methanol and ethyl acetate. GC-MS data of CS revealed the presence of 32 volatile organic compounds (VOCs); mostly fatty acids, poly phenols and aldehydes in its crude sample and 45 VOCs in the aqueous extract, out of which 15 VOCs were common in both these samples as predicted by Venn diagram. Furthermore, heat map analysis of GL indicated formation of two clusters: cluster I consisting of aqueous extracts (A1 and A2) and cluster II consisting of methanolic (M1 and M2) and ethyl acetate (EA1 and EA2) extracts. It demonstrated close relatedness among fruiting body and mycelium fractions of each extract type, i.e., aqueous, methanolic and ethyl acetate but the colour intensity of each grid depicted the quantitative variability in terms of bioactive metabolites.

The present study clearly illustrated the richness of medicinal mushrooms in VOCs that have reported nutraceutical as well as pharmacological properties.

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P-26

Raman spectroscopic studies of labdane diterpene, a bioactive compound from the seeds of *Alpinia nigra*

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Abstract: A wide range of bioactive compounds have been isolated and studied from the genus *Alpinia* [1], however, limited literature is available on *Alpinia nigra* and its phytochemicals [2]. Naturally occurring bioactive compounds have been characterized extensively using a number of analytical techniques [1]. One such compound previously isolated from the mature seeds of *A. nigra* is labdane diterpene, (E)-labda-8(17), 12-diene-15, 16-dial, having diverse biological attributes [3]. Structural elucidation of labdane diterpene was done by HR-MS, FTIR and NMR [4]. In the current study, the compound is extracted from the moderately mature seeds of *A. nigra* by hot solvent extraction using hexane and further isolated by column chromatography. Moreover, the chemical and structural information of isolated compound was obtained by Raman spectroscopy and its optimized geometry was also correlated with theoretical calculations using density functional theory (DFT) which provide a source of accurate normal mode assignment. The study also includes surface enhanced Raman spectroscopy (SERS) after conjugation of the compound with copper nanoparticles. SERS showed strong and intense enhancement in the characteristic weak Raman bands of the compound which helps in its easy identification and discrimination from a mixture of compounds.

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P-27

Molecular modeling studies on heat shock protein as possible antiviral target

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The 90kDa Heat shock protein (Hsp90) is molecular chaperone, which due to its unique and flexible structure interacts with a wide range of substrates and client proteins including kinases and transcription factors. The protein which is highly conserved in eukaryotes governs many cellular processes including cell growth, apoptosis, RNA processing, evolutionary diversification and stress responses[1]. The ATPase activity of the protein regulates the interaction of Hsp90 with the diverse clientele[2].

Here we report a 3D structure model using a potential compound NVP-AUY922to delineate the molecular basis of Hsp90 and its binding phenomenon. The N-Terminal domain were found interesting region and flexible docking studies at the ATP binding siteprovided understanding about ligand binding. The docking studies correlated well with the inhibitory activity of the molecules. To further study the structure activity relationship and determine what affect our most active compounds has on the ATP binding site, we performed 10ns Molecular Dynamic simulations of protein ligand complexes using Desmond[3, 4]. We analyzed the simulations of the molecule with highest activity and compared the secondary structure changes in the ATP lid with those obtained in the trajectory run of AUY922 and ATP.

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P-28

Homology Modeling and Docking Study on Filariasis DHFR protein

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Abstract: A systematic technique for protein modeling offers great assistance in the study of protein function, dynamics, interactions with ligands, other proteins and even in drug discovery and drug design [1]. Subcutaneous filariasis is rare parasitic disease caused by *Loa Loa* (eye worm) and *monosonallastreptoscerca species.* In our approach we have used knowledge based homology modeling to developthree dimensional structure of dihydrofolate reductase present in *Loa loa* species.The procedure involves alignment that maps residues in the query sequence to residues in the template sequence to generate structural model of target [2], which was further refined and validated by Ramachandran plot. Finally the derived model was employed to perform, for the first time, docking simulation on identified protein structure, revealing a new useful paranoma to be exploited for the further development of new drugs to treat diseases.

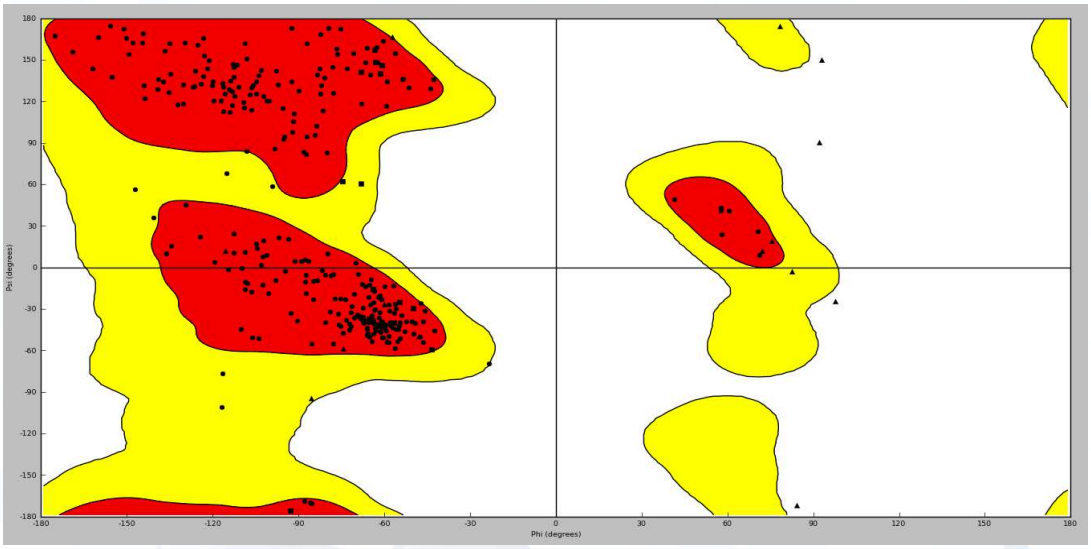

Fig. 1.: Ramachandran Plot of identified protein structure

Keywords: DHFR, Filariasis, homology modelling

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P-29

Development of pyranone carboxamide analogs as anti-HCV molecules

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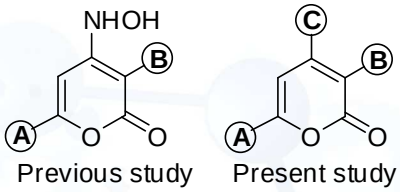
The discovery of new non-nucleoside antiviral compounds is a significant and growing for treatment of viral infections. In our previous study, we found that α-pyranone carboxamide analogs with **A** as phenyl, **B** as substituted phenyl and **C** as 4-NHOH were significantly potent which supports our current results (A, B & C : Figure 1). In addition, furan-2-yl moiety (**A**) was evaluated with phenyl/substituted phenyl (**5a-k**) and found to be equally good as phenyl (**A**), specially (**5g**). In the current study, we present a synthetic exploration for the study of new α-pyran scaffold "4-hydroxyamino-α-pyranone carboxamide" & "4-hydroxyethylamino-α-pyranone carboxamide" as promising anti-HCV agents. A comprehensive structure activity relationship (SAR) was explored with twenty nine synthesized compounds. In particular, one compound (**5g**) demonstrated potential anti-HCV activity with (EC_{50} = 0.27 µM) in cell based HCV replicon system with lower cytotoxicity (CC_{50} > 20 µM) from the current studies. Further investigations, including biochemical characterization are yet to be performed to elucidate its possible mode of action.



Keywords: Non-nucleoside inhibitors, α-pyranone carboxamide analogs; hepatitis C virus; structure activity relationship.

P-30

Synthesis and applications of porphyrin - pyrene conjugates by click reaction

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Huisgen-sharpless-meldal (HSM) reactions are important reactions with high selectivity. The scope of the reaction of terminal acetylene and substituted azide in natural products, bioconjugates, supramolecular chemistry polymes, material chemistry and photodynamic therapy is huge. The copper- catalysed alkyne – azide cycloaddition reaction is unique building block for the synthesis of 1,4-disubstituted 1,2,3 – triazoles. The 1,2,3- triazole moiety is versatile ion recognition unit for both cations and anions. The nitrogen containing lewis based ligands to coordinate with different transition metals cations. Several triazole derivatives recognize anions through a cooperative triazole C-H-anion hydrogen bonds. Pyrene[1] is a spatially sensitive probe that displays an ensemble of monomeric fluorescence emission peaks (375 – 405 nm), and an additional band (called excimer) at ~460 nm when two fluorophores are spatially proximal. The high fluorescence quantum yield and monomer to excimer emission of pyrene is very sensitive to minor change in microenvironment for the development of chemosensor. Pyrene form excimer and monomer and is an important fluorogenic units. Various porphyrin based donor-acceptor systems have been synthesized covalently / non covalently linked to either an energy donor or an acceptor to study the intramolecular electron transfer and energy transfer reactions. The energy or electron acceptors such as fullerenes at pyrrole β-position of porphyrins have been reported however energy or electron transfer at pyrrole β-position of a porphyrins are less studied. Hence selected porphyrin-pyrenes by triazole as linker have been synthesized and their photophysical reactions have been examined in different reaction conditions with the aim of development of newer materials. If both the parts have conjugated structures, the triazole moiety acts as a better linker thanthe conjugated linkers in terms of facilitating charge transfer and electronic communication between the two parts. Thus porphyrin-pyrene[2] conjugates linked via triazole moiety by following click chemistry have been synthesised. By varying the spacer between the porphyrin and pyrene moiety the photophysical properties seem to change thus various conjugates with different spacers have been synthesised. Also the binding of the conjugated with different ions has been studied through UV-Visible and fluorescence spectroscopy.

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P-31

Compound profiling of thiophene analogues as anti-inflammatory COX-2 selective inhibitors through virtual screening

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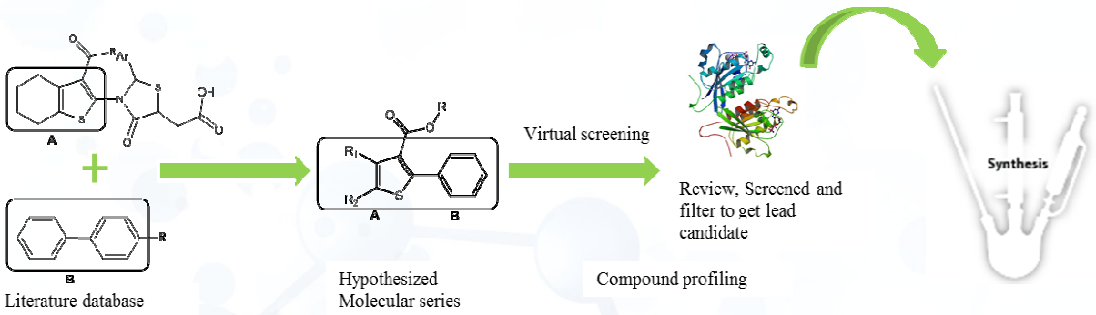
Abstract: To treat inflammation classical non-steroidal anti-inflammatory drugs (NSAIDs) widely used. NSAID act by inhibiting the COX enzyme, it decreases formation of thromboxanes, prostaglandins and produce analgesic and anti-inflammatory effect.[1]Cyclooxygenases (COXs) are membrane-bound heme proteins and have two distinct isoforms, COX-1 and COX-2.[2] Classical NSAIDs nonselectively inhibit both the isoform and cause gastric failure like bleeding and ulcer.[3] In order to prevent these side effects, current strategy of COX-2 selective NSAIDs improved the gastric safety profile. Several COX-2 selective drugs are reported but they are having cardiovascular side effect.[4]. Therefore, the discovery of new safer anti-inflammatory drugs with COX-2 selectivity represents a challenging goal to the researchers of this field.



It has been reported in the literature that compounds having substituted thiopheneheterocycle exhibited potent anti-inflammatory activity and further literature review revealed that biphenyl scaffold is an integral part of NSAID like flurbiprofen.For present study; molecules with integral molecular features of both, substituted thiopheneheterocycle and biphenyl scaffold which attached to another aromatic ring by a linker moiety; have been designed and evaluated by virtual screening tools. Docking study showed that designed molecules and celecoxib have similar type of interaction with COX-2 active site; common interacting residues are: Arg499, Phe504, Ser339, leu338, Arg106 and also have comparable glide score to celecoxib. Thiophene based biaryl has been well adopted in hydrophobic pocket and arylsulfonamide group is favored in hydrophobic pocket ofCOX-2 receptor binding site.Due to bigger size of molecules, none of a single molecule docked on COX-1 active site which is small than COX-2 active site.

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P-32

Sulfated fullers earth: a new solid heterogeneous catalyst for amide synthesis

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Abstract: The amide bond is widely prevalent in both naturally occurring and synthetic compounds. As many as 65% of drug molecules prepared by leading pharmaceutical companies contain an amide unit, indicating its importance and prevalence in synthetic organic chemistry.[1] Formation of amides usually involves Activation of carboxylic acidsby forming acid chlorides,[2] anhydrides or esters requires a separate step and this protocol suffers from low atom economy. Although there are a large range of reagents and strategies for amide bond formation available,[3] few can really be considered ideal. Currently there is a focus on the development of novel, atom-economical, benign methods for amidation.

Amide formation avoiding poor atom economy reagents is a priority area. We have synthesized sulfated fullers earth asa new reusable and environmentally benign heterogeneous catalyst for direct amide formation between carboxylic acid and amine.

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P-33

Synthesis of N-Substituted 4-Aminoquinoline-Pyrimidine Hybrids as Potential Antimalarial and Anticancer Agents

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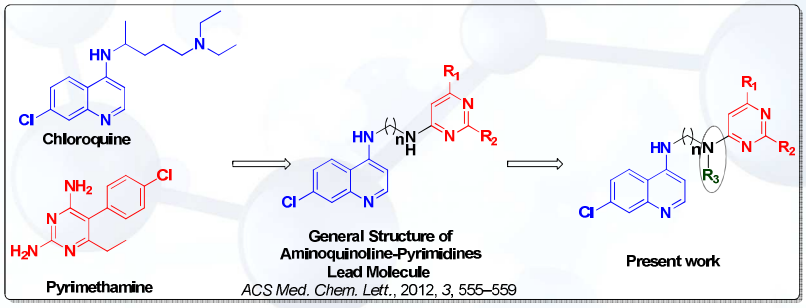
Artemisinin-based combination therapies (ACTs) have been recommended by the World Health Organization (WHO)for first-line treatment against*Plasmodium falciparum* malaria and have largely replaced drugs such as chloroquine and sulfadoxine-pyrimethaminedue to the widespread parasite resistance especially in sub-Saharan Africa[1]. However, recent reports of artemisinin resistant strains of *Plasmodium* emerging in some malaria endemic areas of South East Asia continue to raise concerns over the long-term efficacy of ACTs and have increased the urgency to discover and develop new drugs [2].Several approaches have been made towards the development of new antimalarial agents to address the problem of drug-resistance and the concept of molecular hybrids has shown promising results. In hybrid antimalarials, two (or more) discrete antimalarial scaffolds are linked covalently, usually through a spacer, in an anticipation that these compounds may act by inhibiting simultaneously two (or more) different conventional targets[3]. Compounds containing 4-aminoquinoline pharmacophore are well known to show antimalarial and anticancer activities [4-6].A class of hybrid molecules consisting of 4-aminoquinoline and pyrimidine nuclei were synthesized and tested for antimalarial activity against both chloroquine (CQ)-sensitive (D6) and chloroquine (CQ)-resistant (W2) strains of *Plasmodium falciparum* through an*in vitro* assay. Some hybrids showed good antimalarial activity against both CQ-sensitive and CQ-resistant strains of *P. falciparum*.Aminoquinolines such as chloroquine and other related antimalarials were also known as multidrug resistance reversal (MDR) agents in cancer chemotherapy[7-8].Therefore representative analogues were also tested on NCI 60 cancer cell line panel and showed cytostatic potential at sub-micromolar concentrations against several cell lines specially against leukemia.



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P-34

Computer Aided Drug Design of Innovative TNFR1 modulator as Anticancer Agent

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Abstract: Cancer remains one of the leading causes of morbidity and mortality worldwide. It is predicted that by 2020, the number of new cases of cancer in the world will increase to more than 15 million, with deaths increasing to 12 million. Much of the burden of cancer incidence, morbidity, and mortality will occur in the developing world.[1]Tumor necrosis factor-α (TNF-α), an important cytokine produced by activated monocytes/macrophages, was originally identified as an endotoxin-induced serum factor that causes hemorrhagic necrosis of transplanted solid tumors. This cytokine is involved in the regulation of a wide spectrum of biological processes, including cell proliferation, differentiation, apoptosis, lipid metabolism, and coagulation. [2]In contrast to chemotherapeutic drugs TNF specifically attacks malignant cells, and mediates cell destruction by direct cell-to-cell contacts. [3] TNF can bind to two receptors, TNFR1 and TNFR2. [4]

As most information regarding TNF signaling is derived from TNFR1 it is selected as target.Active binding site of the receptor was determined using site map analysis. Interacting peptide of TNF was docked with active site of TNFR1. Based on the docking study selected peptides were converted into peptidomimetics and further into non-peptidomimetics. These non- peptidomimetics were transformed into drug like new chemical entities following Lipinski rule of five.TNF-α exhibits striking cytotoxicity selectively against various tumor cells hence, it has attracted attention as a potential antitumor drug.

Keywords: TNFR1, TNF-α, Anticancer, Computer Aided Drug Design

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P-35

Highly active cobalt oxide nanoparticle on Alumina-Silica support for the synthesis of 2-phenyl benzimidazoles

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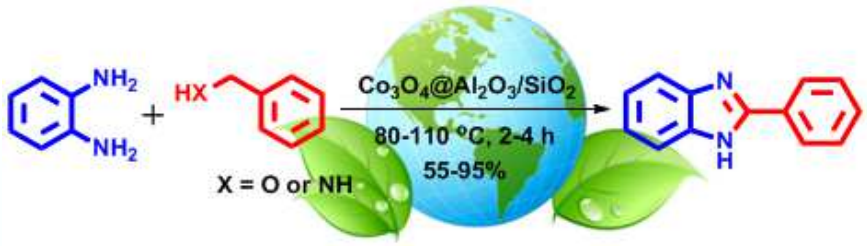
Abstract: Benzimidazole derivatives have significant importance in the synthesis of natural products, pharmaceuticals and fine chemicals. These compounds have been explored to a vast extent because of their biological activities as antitumor agents Chu et al. [1]and enzymeinhibitors Kim et el [2]. The traditional method for the synthesis ofbenzimidazoles is coupling of ortho-arylenediamineswith carboxylic acids or their derivatives at strong acidic and high temperatures (> 200 ^{o}C).The other method is the oxidation of benzimidazolineintermediates that are generated from the condensation ofortho-arylenediamines and aldehydes. This method producesbenzimidazoles at relatively low temperatures, but requires unstable aldehydes as reactants andstoichiometric or excess amounts of strong oxidants such asDDQ (2,3-dichloro-5,6-dicyano-1,4-benzoquinone)Chang et al. [3]. Recentadvances in this method have allowed the use of molecularoxygen as an oxidant Chen et al. [4], but these processes require homogeneouscatalysts.Alternative methods that precede under mild reaction conditionswith stable reactants, such as alcohols and carboxylic acids and easy-to-handle heterogeneous catalysts are desirable for economically and environmentally benignbenzimidazole production.

The cobalt oxide nanoparticles on alumina-silica support were prepared by impregnation method and applied for the synthesis of benzimidazoles from benzyl alcohols and benzyl amines with*O*-phenylene diamines.The characterisation of nano Co_3O_4 on Al_2O_3/SiO_2 matrix was studied byXRD, XPS, TEM, SEM, VSM, ICP-AES and BET-surface area. To our delight the catalyst prepared in this method has given excellent yields for the synthesis of gram scale preparation of benzimidazoles and the robustness ofthe catalyst was examined by reusing it for five consecutive runs.



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P-36

STUDIES ON THE MOLECULAR INTERACTIONS OF CARDIAC ANTI-ARRHYTHMIC DRUG NAMELY PROCAINAMIDE HYDROCHLORIDE IN WATER USING VOLUMETRIC AND ACOUSTIC APPROACHES

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In continuation to our study of biologically important compounds [1-4], in this paper we are reporting the data of densities and speeds of sound of the Cardiac Anti-arrhythmic Drug namely Procainamide Hydrochloride (Figure 1) in water rich region at different temperatures in the range of T = (298.15–318.15) K under atmospheric pressure. From the experimental density (ρ) and speed of sound data (u), different derived parameters such as apparent molar volume (ϕ_V) of solute, partial molar volumes (V_i), isentropic compressibility (β_S), apparent molar isentropic compressibility (ϕ_{KS}) at different temperatures have been calculated, and the results have been interpreted in terms of different hydrophobic and electrostatic interactions. The limiting properties such as limiting partial molar volume ($\overline{V}_i^0$), limiting apparent molar isentropic compressibility (ϕ_{KS}^0), temperature derivative of limiting apparent molar isentropic compressibility ($d\phi_{KS}^0/dT$), etc. for all the binary mixtures have been obtained. The results have been interpreted in terms of various interactions among solute and solvent molecules such as hydrogen bonding, (solute + solute) and (solute + solvent) interactions and structure making and structure breaking tendencies of the solutes in water.

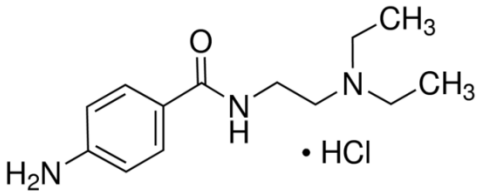

Figure 1. Structure of **4-Amino-N-(2-diethylaminoethyl)benzamide hydrochloride, 4-Aminobenzoic acid 2-diethylaminoethylamide i. e.** Procainamide Hydrochloride

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P-37

Improved Synthesis of *meso*-Aryl-Substituted [26]Hexaphyrins

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Expanded porphyrins have recently emerged as an intriguing class of functional molecules in light of their interesting optical, electrochemical, and coordination properties.[1] *meso*-aryl-substituted [26]hexaphyrins can be regarded as real homologues of porphyrin in terms of the conjugated cyclic π-system with alternate arrangement of pyrroles and methine carbon atoms.[2] [26]Hexaphyrin is an attractive molecule in view of the relatively high yield, the intense absorption band in the visible region, and pronounced aromaticity that arise from the 26-π circuit. The meso position of these compounds can be readily functionalized with polyaromatic hydrocarbons. Lindsey method for the synthesis of *meso*-aryl-substituted expanded porphyrins involve strong acid like BF_3OEt_2 followed by oxidation with DDQ. A newer method has been developed using sulfonated graphene, which serves as a solid carbocatalyst. The solid acid has been synthesized by diazotization of reduced graphene oxide [3] and by refluxing reduced graphene oxide in conc. sulphuric acid. The synthesized compound posess unusual electronic properties of these expanded π-systems make them interesting for a variety of applications including photodynamic therapy, two-photon absorption, nonlinear optics, organic semiconductors and photovoltaics.

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P-38

Identification and optimization of Aminoquinoline based hybrids as Potent Nurr1 Agonists for the Treatment of Parkinson`s Disease

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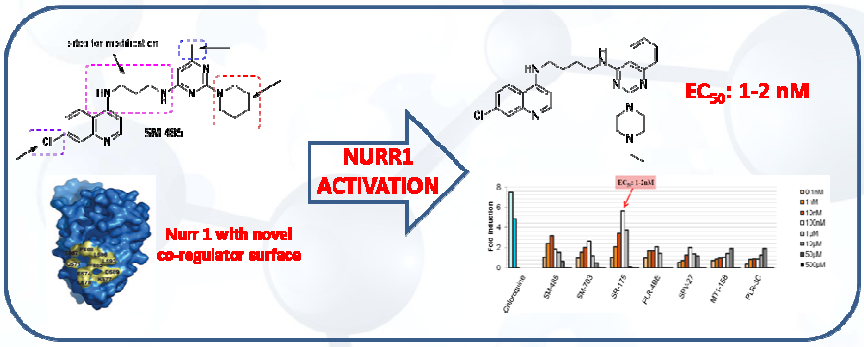
Parkinson disease (PD) is themost prevalent chronic movement disorderand the second common neurodegenerative disorder caused by the selective degeneration of midbrain dopamine generating neurons, affecting approximately seven million people globally. Presently, there is no cure for PD but a variety of medications provide for symptomatic treatments (e.g. L-DOPA), which lose their efficacy over time, with associated severe side effects[1]. Thus, there is a cogent need to develop mechanism-based and/or disease modifying treatments for PD. Recent studies indicate that the orphan nuclear receptor Nurr1 is essential for the development and maintenance of midbrain dopaminergic neurons[2,3] and also for their protection from inflammation-induced death suggesting it as a promising target for the development of novel disease-modifying therapeutics for PD[4]. It does not possess a cavity for ligand binding but recently a novel hydrophobic interaction surface was identified that could serve as a molecular target for Nurr1 activating compounds. To address this possibility, a high-throughput assay system based on Nurr1's ability to directly activate tyrosine hydroxylase promoter function was established, which resulted in the identification of 4-amino-7-chloroquinoline scaffold as a potent Nurr1 activator. Moreover, linking this scaffold to various hetero-aromatics led to aminoquinoline-pyrimidine conjugates [5,6] as promising Nurr1 agonists for the development of novel therapeutics for PD. Further diversification to understand the SAR and optimization led to Aminoquinoline-Quinazoline hybrid SR-175 having EC_{50} value 1-2 nM range withfive-fold induction of Nurr1.



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P-39

Novel route for synthesis of Raloxifene

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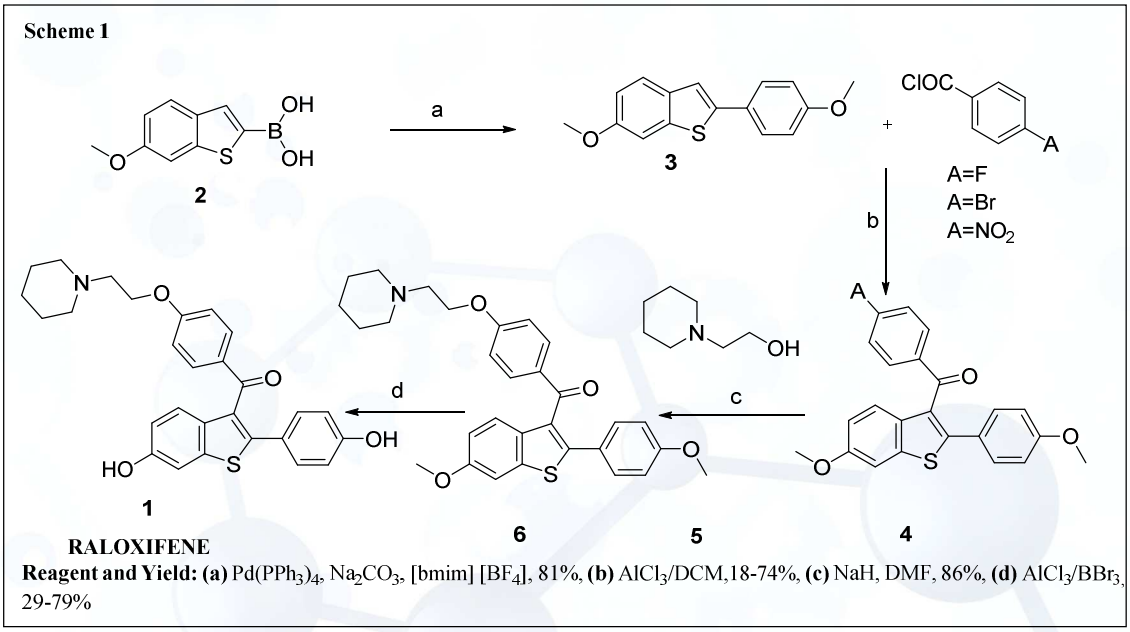
Abstract: Selective estrogen receptor modulators (SERM) are a class of therapeutic agents widely prescribed for the treatment and prevention of breast cancer, osteoporosis, and postmenopausal symptoms. [1] Raloxifene, an example of oral SERM is prescribed primarily for the treatment and prevention of postmenopausal disorders in woman. [2]

Present work deals with synthesis of various raloxifene intermediates by novel method.

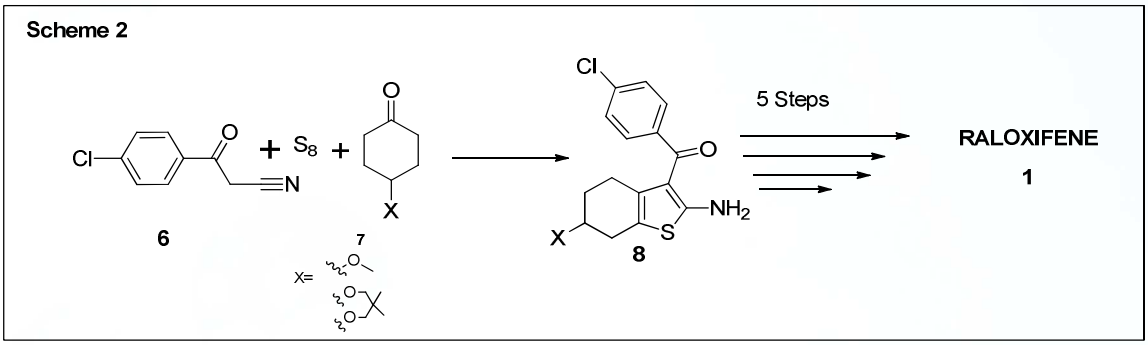
Literature routefor synthesis of Raloxifene:



The biaryl,**3**was synthesized from boronic acid, **2**bySuzuki coupling reaction (Scheme 1) . Ketone**4**was obtained by Friedel crafts acylation at 3positionfrom compound**3**[3].Followed by base catalyzed condensation of 4 with **5** to obtain compound **6**. Demethylation ofcompound **6**to obtain raloxifene**1**[4].Literature method have low overall yield due to multistepand use of transition metal catalyst. Which make the method commercially non-viable with cost considerations. Hence, there was need to develop new alternative route with to reduce cost of raw material/reagent with improve overall yield and reduced number of steps.

Novel method for synthesis of Raloxifene:

Gewald product **8**, was synthesized by three component condensation of commercial available active methylene **6**, ketone 7 and sulphur under Gewald conditions (Scheme 2) [5]. Product **8** was N, N-dialkylated, followed by coupling with (piperidin-1-yl)ethanol, deprotection of **X** group and aromatization with oxidizing agents. The product obtained was demethylated to obtain raloxifene **1**. Identity and purity of each intermediate was ascertained byMP, TLC, FTIR, ^{1}H NMRand MS.



Keywords: Raloxifene, Selective estrogen receptor modulators (SERM), Process chemistry

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P-40

X-ray Crystal structure studies of Methyl 2-(4-(allylamino)-2-oxo-6-phenyl-2*H*-pyran-3-carboxamido) acetate

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Single crystal X-ray diffraction analysis of our compound reveals the π-π stacking interaction in a non-aromatic coplanar system of solid-state assembly.

The compound form zigzag assembly through π-π stacking interactions supplemented by strong N-H…O intermolecular interactions. The offset stacking among non-aromatic pyran-2-one ring and aromatic phenyl ring is the special feature of our crystal structure. The planarity of compound along with the π-π stacking gives a staircase- like arrangement to an individual chain. A chain is connected to other through strong double N-H…O/O…H-N hydrogen bonding interactions forming zigzag assembly. These strong interactions are similar to the base pairing interactions in DNA. Owing to the similarity with interactions in DNA, this structure may serve as a model to understand the interactions in DNA. Overall study reveals: a) π-π stacking interaction is shown between a phenyl ring and a non-aromatic 2H-pyran-2-one ring. Mostly π-π stacking interactions are observed in aromatic π-conjugated systems but stacking between an aromatic and non-aromatic system is either not observed or rarely reported in the literature; b) The intramolecular C-H…O interaction make the two rings planar with a dihedral angle of 11.1°. c) An additional factor is the weak C-H…O interactions leading to the crystal lattice stabilization.*(Authors acknowledge to Department of Science & Technology (DST), UGC and BIT Mesra for research grant support)*

P-41

A Rational Approach to Design Imidazole based Ionic Liquids as Anthelmintic Leads

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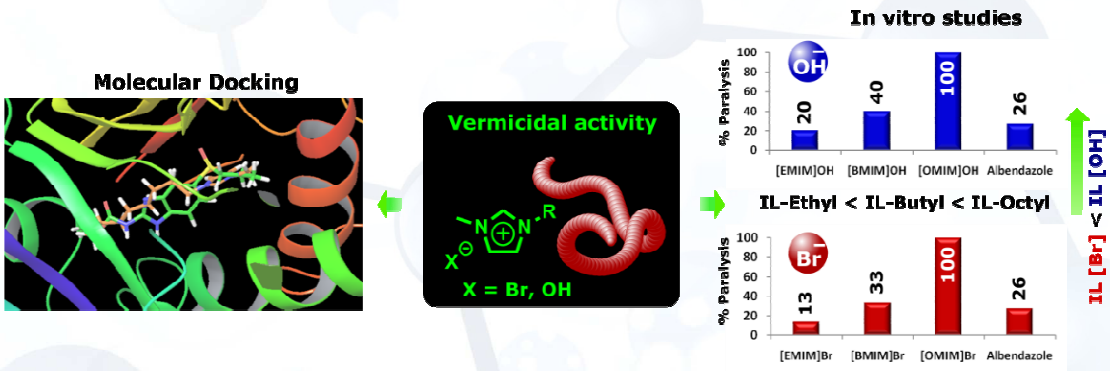
A series of imidazolium derive different ionic liquids (ILs) of the kind 1-alkyl-3-methylimidazolium bromide/hydroxide (IL-Br and IL-OH) tailored with different N-alkyl side chains (-C_8H_{17}, -C_4H_9, -C_2H_5) were synthesized and evaluated for their vermicidal activity against the Indian earthworm, *Pheretima posthuma*. The percentage of paralysis and mortality of earthworms against ILs were recorded in a dose and time dependent manner. As the N-alkyl side chain length increased from -C_2H_5, -C_4H_9, and -C_8H_{17} in both IL-Br and IL-OH, an increase in vermicidal activity was noticed (IL-C_8H_{17}, IL-C_4H_9> IL-C_2H_5). Also, IL-OH exhibited a significant vermicidal activity compared to IL-Br. Hence, it is obvious that the vermicidal activity of ILs is strongly dependent on the nature of the N-alkyl side chain length as well as the counter anion. [OMIM]OH showed higher activity than the remaining ILs and the standard anthelmintic drug, Albendazole.The above discussed experimental findings (in this para) were in good agreement with the molecular docking studies, which clearly explained the influence of the extended alkyl chain associated with the imidazolium scaffold on the binding affinity between the ILs and the β-tubulin receptor.This investigation presents imidazolium-based ILs as a potential group of anthelmintic agents and we envisage that they may find possible therapeutic application in the control of helmintic infections. These initial results encouraged us to pursuit our research further in this line by taking different combinations of heterocyclic fused rings with different possible anions to improve their pharmacokinetics and pharmacodynamics s well as their toxicity.



P-42

Synthesis and Antimalarial Activity of Novel 1, 2-dioxa-4-aza-indenones and 1, 2-dioxa-4-aza-fluorenones

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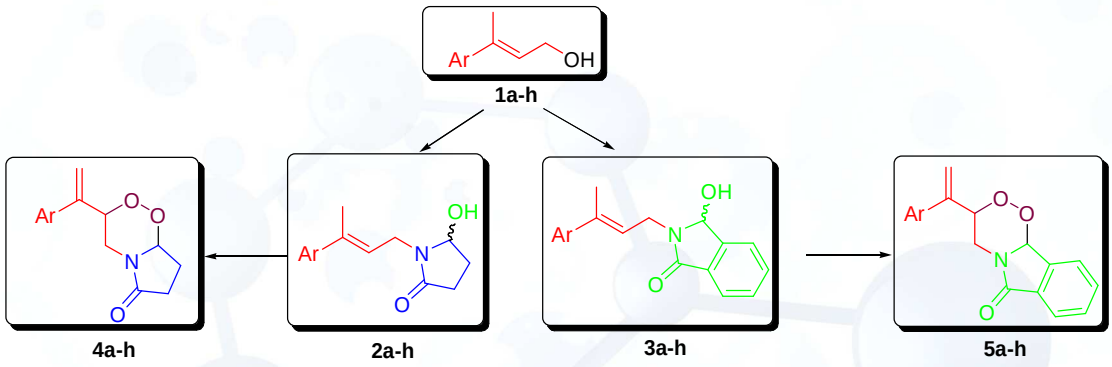
For the first time, novel 1, 2-dioxa-4-aza-indenones **3a-h** as well as 1, 2-dioxa-4-aza-fluorenones **5a-h** were synthesized using $^1O_2$-mediated photo-oxygenation methodology as key step in 52-71% yields from easily accessible starting materials **2a-h** and **3a-h** respectively which in turn can be obtained from allylic alcohols **1a-h**, in which one of the oxygen atom of 1,2,4-trioxane ring has been replaced by nitrogen atom. The methodology is simple and is an efficient way to access 1, 2-dioxa-4-aza-indenones and –fluorenones. All these compounds were assessed for their *in vitro* antimalarial activity against *Plasmodium falciparum.* Compound **5a**, **5c** and **5f**, the most active compound of the series, showed IC_{50} values of 9.43, 8.83 and 5.63 ng/ml, respectively which was found to be comparable to that of antimalarial drug Chloroquine (IC_{50} value 5.2 ng/ml).



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P-43

Development of Glyco *bis*-peptide Cationic amphiphiles for Antileishmanial Activity

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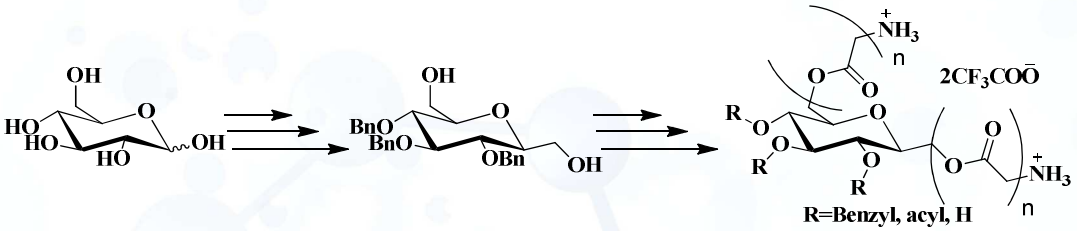
Cationic amphiphiles contain positively charged amino functions define a structurally diverse class of antibacterial, antimicrobial, and antiprotozal with broad spectrum activity and different mode of action. It is generally believed that the amphiphilic topology is essential for insertion into and distruption of cytoplasmic membrane. In the present work, we have prepared a novel class of cationic amphiphiles termed as Glyco *bis*-peptide which has been decorated with hydrophobic residue in the form of long chain acid, peptide chains as hydrophilic domain connected via sugar molecule. Owing to the presence of cleavable ester moiety, these new amphiphiles are hydrolysed spontaneously at physiological conditions. This property enables them to be readily metabolised and therefore, they have potential to be superior antibacterial, antimicrobial, and antiprotozal. The synthesized analogs were evaluated for In-vitro antileishmanial activities. The screened molecules show promising results, thus proving as good scaffolds for the synthesis of different antileishmanial agents.



Scheme: Synthesis of glycine loaded Glyco *bis*-peptide amphiphiles.

Detailed synthetic scheme will be presented during the poster session.

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P-44

Synthesis of amide derivatives of 7-substituted coumarin derivatives and their biological applications

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Cancer is a fatal disease after cardiovascular in terms of morbidity and mortality affecting human health worldwide [1].On-going research in this area has developed effective routes to treat it. At the same time, drawback to get effective treatment for such a deadly disease is limited medicines. Due to this, scientific researchers and commercial bodies are trying their best to discover anticancer drugs with good potency, safety and selectivity [2-4].Synthetic coumarin derivatives have been reported with wide range of biological activities along with beneficial effects on human health.In continuation of our work on synthesis of coumarin derivatives as anticancer and antimicrobial agents [5],we report herein synthesis of amide derivatives of 7-substituted coumarins and their screening for anticancer activity.

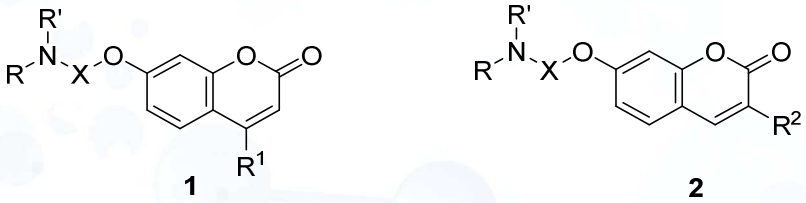

Figure 1: Derivatives of 4-substituted-7-alkoxy coumarinand 3-substituted-7-alkoxy coumarin.

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P-45

Design and synthesis of 4-aminomethyl benzocoumarin derivatives asantidiabetic agent

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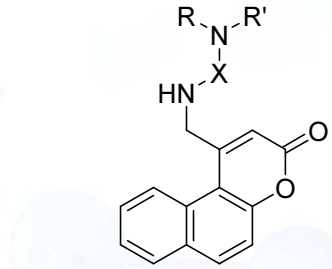
DPP-4 inhibitors are new class of compounds for treatment of Type 2 diabetes and several drugs have been recently approved in this class such as sitagliptin, vildagliptin [1-2].All these compounds have started showing one or another kind of side effects during the development studies [3-4].The mode of action for DPP-4 inhibitors is to increase levels of GLP-1 and GIP *via* inhibiting glucagon levels which in turn increases insulin secretion and decreases blood glucose levels. Novel coumarin derivatives containing amide linkage or small peptide linkage with natural/ unnatural amino acids as antidiabetic agents have been reported from my group [3-4]. In continuation of our work on synthesis of coumarin derivatives,we report here design and synthesis of 4-aminomethyl beznocoumarin derivatives(Figure 1) and antidiabetic activity.



X= linkage
R,R'= H, alkyl, aryl, part of heterocyclic ring

Figure 1: Derivatives of 4-aminomethyl beznocoumarin

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P-46

Synthesis and characterization of some new functionalised, oxazole containing compounds and their anticancer activity

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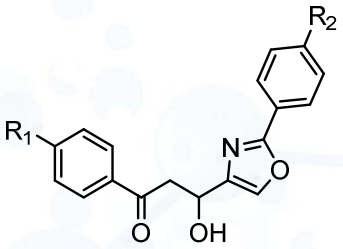
Medicinal chemistry is an interdisciplinary science creating the inter-phase between chemistry and life science.A number of oxazole containing natural products have been isolated and characterized in recent years[1,2]. They are oxazole containing macrolides isolated mostly from marine source. The fascinating biological activities of these oxazole alkaloids have prompted the synthetic chemist to undertake their synthesis[3]. As heterocyclic compounds have close association with biological activity of molecules and with medicinal chemistry[4,5], we have been interested in study of oxazole chemistry and their applications and also look forward to continuing exploring the chemistry of new heterocyclic entities. In this direction, some new β-hydroxy ketones **1**, which are otherwise difficult to isolate, have been synthesised, isolated and characterised, and have been converted to the corresponding aryl-oxazolyl chalcones **2** with an intention to study their biological activity and explore their chemistry for the synthesis of new substituted heterocycles.



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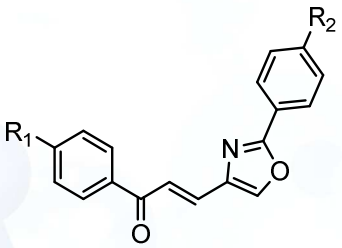

2

R_1 = F **R_2** = H, Cl, Br, F, CH_3, OCH_3, NO_2

As the newly synthesised compounds contain oxazole with □-hydroxy carbonyl functionality and the oxazole moiety conjugated with the carbonyl group on the linker chain in their structure, they have been screened for anticancer activity. Anticancer activity of the newly synthesised compounds has been carried out at NCI (National Cancer Institute), USA using 60 types of human tumour cell lines of 9 different kinds of cancers. The chemistry and activity results will be presented.

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P-47

Growth and challenges of Indian pharmaceutical industry

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The Indian pharmaceutical industry is one of the most attractive investment destinations in the world. With ever increasing returns, lowering risks and anticipated multifold growth, investors are more interested in this industry than ever before. India has become a prime destination for manufacture of branded generic medicines.

From its nascent stages in the 1970s, the Indian pharma industry has become a mature industry. While, the industry was previously known for manufacturing generic drugs, the industry dynamics have now undergone a sea of change. Presently, the Indian pharma industry stands diversified into various spheres of activities including research and development (R&D), manufacturing of branded, generic and branded generic drugs, manufacturing APIs, laboratory testing and clinical research. The Indian pharma industry ranks fourth in terms of volume and 13th in terms of value globally.

Developments in the health insurance, medical technology and mobile telephony, local pharmaceutical R &D sector can serve as key driver of economic growth, this will help increase income levels and improve the access to healthcare services in India The core challenges faced by pharma industry are the drug price control, regulatory reforms, quality management and conformance to global standards but with public-private partnerships these hurdles could be overcomed. This article reviews the growth, development and challenges faced by Indian pharmaceutical industry.

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P-48

Recent trends in nanotechnology and nanoscience

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Abstract: Nanotechnology and Nanoscience have become the most interesting and exciting fields in recent years. The synthesis of gold nanoparticles in non polar organic media is a new area of research. With the awareness of green chemistry, the need to develop eco-friendly synthesis protocols that do away with the use of toxic chemicals becomes important. In this direction and bio-related processes that use microorganisms such as bacteria, fungi and actinomycete have been developed to grow nanocrystals of silver and gold both inside and outside the biomass. Nanosized semiconductors have been extensively investigated due to their special electrical and optical properties in fabricating nanoscaled electronic and optoelectronic devices.

Keywords: Nanoscience, Nanotechnology, eco-friendly synthesis.

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P-49

Synthesis, characterization and enantiomeric recognition of new chiral pseudo-peptide metal complexes: DNA binding, cleavage, Topo inhibition and potential chemotherapeutic activity against human cervical cancer cell line

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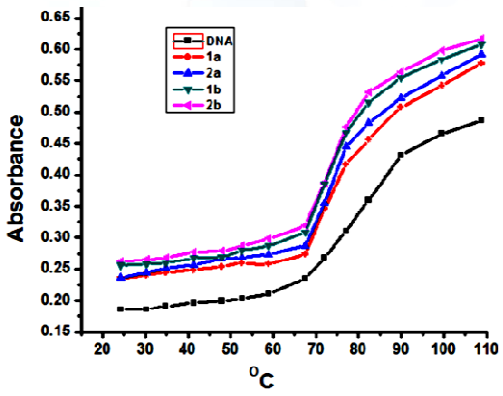
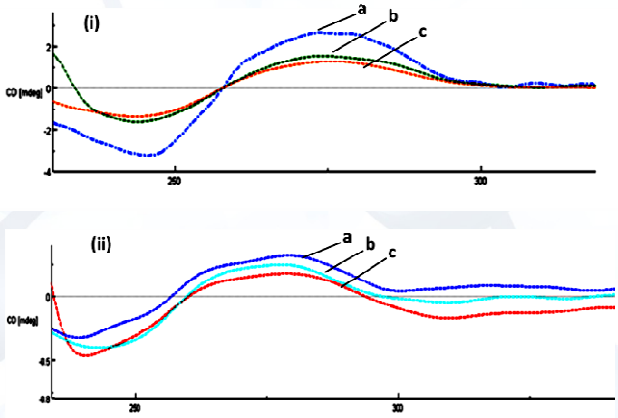
Abstract: New Cu(II) and Zn(II)-based pseudo peptide complexes (**1_S**, **1_R**) and (**2_S**, **2_R**) were synthesised from chiral pseudo-peptides of R/S- Phenyl glycinol and N- Methyl iminodiacetic acid. The complexes were thoroughly characterized by elemental analysis, IR, ^{1}H NMR, ^{13}C NMR spectroscopy. *In vitro* DNA binding studies were carried out by UV-vis., fluorescence, thermal denaturation and circular dichroic techniques to ascertain their comparative DNA binding propensity. The extent of binding was quantified by computing their intrinsic binding constant K_b and binding constant K values which revealed that both the S- enantiomers of complexes **1** and **2** exhibited higher binding propensity as compared to their R- enantiomers and magnitude of binding propensity followed the trend **1_S** > **2_S** > **1_R** > **2_R**. The experimental results revealed that the complexes bind strongly to DNA by electrostatic interaction mode and the binding affinity of S-enantiomer of Cu(II) complex with CT DNA was highest in order of magnitude than Zn(II) complexes. Thermal denaturation studies of complexes in the absence and presence of CT DNA were carried out and the calculated ΔT_m was found to be ~3 $^{\circ}$C depicting electrostatic mode of binding corroborated well with the results of UV-vis and flourescence studies. The cytotoxicity profile of **1_S** and **2_S** was studied on human cervical cancer cell line, HeLa by SRB assay revealed significant regression of the cell line with GI_{50} values of <10 µg mL^{-1} as compared to the standard drug Adriamycin. Furthermore, the chemotherapeutic action of drug entities was found to be mediated by Topo enzymatic inhibition.





P-50

Interaction of Tetronic® T1304 micelles with imidazolium based ionic liquids: Investigating the role of counter-ion and chain length

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Abstract: The micellar characteristics of aqueous solution of a star shaped block copolymer T1304(Total mol. wt =10, 500 and % PEO = 40%) have been systematically investigated by cloud point (CP), viscosity, dynamic light scattering (DLS), nuclear magnetic resonance (NMR), small-angle neutron scattering (SANS), and HSDSC measurementsin the presence of several 1-alkyl-3-methylimidazolium (C_nmim^+) based ionic liquids (ILs) varying in alkyl chain lengths in the cation (C_4-C_{10}) and different anions viz. chloride [Cl^-], tetrafluoroborate [BF_4^-], trifluoromethanesulfonate [$CF_3SO_3^-$], hexaflurophosphate [PF_6^-] and octylsuphate [$C_8SO_4^-$].These ionic liquids interact with T1304 micelles in virtue of their hydrophobicity; ILs with hydrophilic counterion (Cl^-) favour demicellization, increase CPand decrease the apparent hydrodynamic diameter (D_h) of micelle while ILs with hydrophobic counterion (PF_6^-) decreases CP and increases the hydrodynamic diameter. Themicrostructural changes on the size/shape of T1304 micelles in the presence of different ILs are explained using SANS. The location of ILs was evaluated from ^{1}H NMR and these results are discussed in terms of the insertion of ILs in T1304micelles. IL molecules with longer alkyl chain penetrate deeper in T1304 micelles. The present study provides valuable information on altering the solution characteristics of T1304 in the presence of ILs that may have industrial applications.

P-51

Enantioselective addition of Cyanide to β-CF_3-β-Disubstituted Nitroolefins: Construction of Trifluoromethylated All-Carbon Quaternary StereogenicCentres

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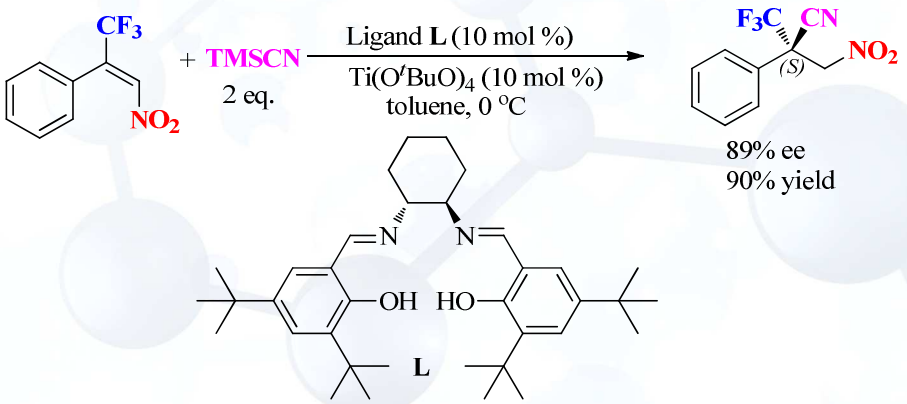
Asymmetric synthesis of compounds bearing all-carbon stereocenter including a CF_3 group is important from the perspective of producing novel bio-active motifs for their commercial exploitation.[1] Such compounds can be readily access by asymmetric cayantion reaction of CF_3-bearing disubstituted olefins.The asymmetric hydrocyanation of trifluoromethylated-β,β-nitroolefins give CF_3-substituted-β-nitronitrile which play a key role in the synthesis of chiral building blocks such as trifluoromethylated-β-amino acids,1,3-amino alcohols, and 1,3-diamines and have a wider application in the pharmaceutical industry. There are only few reports available in literature for the synthesis of chiral β-nitro nitrile by using simple nitroalkenes[2,3,4,5] however none with CF_3 group. In our quest to develop a simple catalytic system for asymmetric cyanation of β,β-disubstituted nitro alkenes our first choice was the use of chiral Ti(IV)salen complexes as catalysts.Thereafter the reactivity of different*in situ* generatedTi(IV) complexes were tested and reaction parameters like catalyst loading, additives, temperature and solvent were optimized. After the successful optimization, *in situ* generated catalyst **[L:Ti(OtBu)$_4$]** (10mol%), using toluene as a solvent at 0^{o}C and this protocol (Scheme 1) was extended for its applicability in various CF_3-substituted nitroalkenes. In all the cases the present protocol gave desired product with good yield (upto 93%) and enantioinduction (upto 89%).



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P-52

Catalytic asymmetric synthesis of α-aminonitrile using Recyclable Chiral Dimeric V(V) Salen Complex

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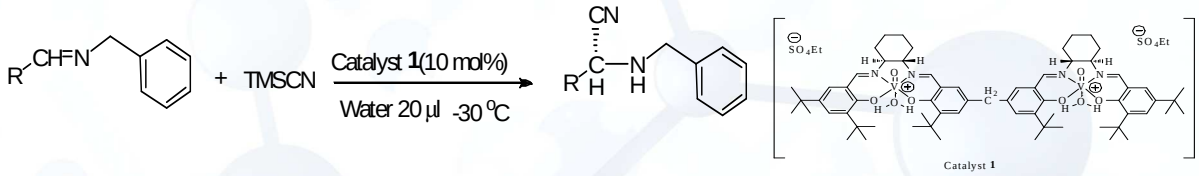
The catalytic asymmetric Strecker reaction is of much importance to modern organic chemistry as it offers a direct and viable methods for the asymmetric synthesis of α-amino acid derivatives.[1] As chiral ligands are expensive, the recycling of chiral catalyst is highly desirable. Our group has been involved in developing recyclable dimeric salen complexes for various asymmetric organic transformations, by fine tuning the solubility of the catalyst by increasing its molecular weight so that the catalyst can be easily precipitated out by hexane in post work up.

Chiral dimeric vanadium (V) salen complex (5 mol%) derived from 5,5-Methylene di-[(*S*,*S*)-{*N*-(3-*tert*-butylsalicylidine)-*N'*-(3',5'-di-*tert*-butyl salicylidene)]-1,2-cyclohexanediamine] with vanadyl suphate followed by auto oxidation was used as efficient catalyst for enantioselective Strecker reaction of variety of aldimines using TMSCN as a source of cyanide at -20 °C. Excellent yield (92%) of *α* aminonitrile and high chiral induction was achieved (*ee* up to 94%) in 10 h. The catalytic system worked well up to four cycles with retention of enantioselectivity.

Table 1. Enantioselective addition of TMSCN to various *N*-benzylimines catalyzed by dimeric V(V) salen complex 1



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P-53

Enantioselective hydrophosphonylation of *N*-benzyl imines, isatin derived ketimines and isatins catalyzed by in-situ generated Ti(IV) macrocyclic salen complexes

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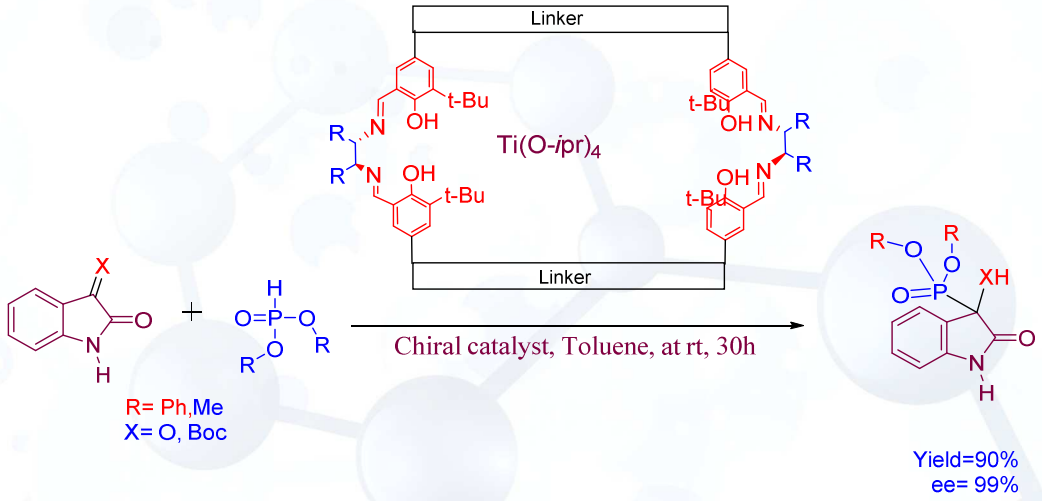
Abstract: Chiral hydrophosphonylation reaction is an important C-P bond formation reaction which results in the formation of various enantiopure bioactive compounds and pharmaceuticals. Though this versatile reaction found its extensive application in addition of phosphite to aldehydes, but still it was not so explored for the less reactive substrates like ketones[1] and ketimines[2] and imines[3]. It is well known in the literature that ketone motif bearing the chiral quaternary carbon center is present in various natural products. In this context, we are interested in developing a recyclable chiral catalyst for the asymmetric hydrophosphonylation reaction of ketones and its derivatives to construct 3-substituted 3-hydroxy structural motif. We have developed a chiral macrocylic Ti(IV) based salen catalyst for the asymmetric addition of phophonates to ketones and imines and found that the catalyst was worked very well at affordable reaction condition and resulted the desired product with good yield 91% and excellent enantioselectivity 99%. And recyclable continually five times with good yield and retention.



Scheme 1, asymmetric hydrophosphonylation of N-benzyl imines isatin, isatinamine

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P-54

STUDIES ON CHELATING PROPERTIES OF FURAN RING CONTAINING ORGANIC LIGANDS

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Abstract: The novel ligand namly,4-(5-((ethyl(methyl)amino)methyl)furan-2-carboxamido)-2-hydroxybenzoic acid (EMFSA) was synthesized by reaction between 5-((ethyl(methyl) amino) methyl)furan-2-yl propionate and 4-amino salicylic acid. The transition metal complexes like Cu^{2+},Co^{2+} ,Ni^{2+}, Mn^{2+} and Zn^{2+} of EMFSA have been prepared and characterized by elemental analyses, spectral studies, magnetic moment determination, molar conductivity measurement and antimicrobicidal activity.

Keywords: 5-((ethyl(methyl)amino)methyl)furan-2-yl propionate,4-amino salicylic acid, spectral studies and Antimicrobial activity.

P-55

SYNTHESIS AND CHARACTERIZATION OF SOME ORGANIC MOLECULES CONTAINING LIGAND

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Abstract: The new ligand 2-hydroxy-4-(methyl((5-(4-sulfamoyl phenyl carbamoyl) furan-2-yl)ethyl amino)benzoic acid (HMSPCFEAB) prepared by condensation reaction between 4-(((5-(ethoxy carbonyl)furan-2-yl)methyl)ethyl amino)salicylic acid and Sulphanilamide was give. It was characterized by elemental analysis and spectral studies. The transition metal chelates Cu^{+2}, Ni^{+2}, Co^{+2}, Mn^{+2} and $Zn^{+2}$of HMSPCFEAB were prepared and characterized by metal to ligand ratio, IR spectra and reflectance spectroscopies and magnetic properties. The antifungal activity of HMSPCFEAB and its metal chelates was examined against various fungi.

Keywords: Sulphanilamide, 4-(ethylamino) salicylic acid, Magnetic moment, Spectroscopies study and Antifungal properties.

P-56

Enantioselective syntheses of β-amino alcohols catalyzed by recyclable chiral Fe(III) metal complex

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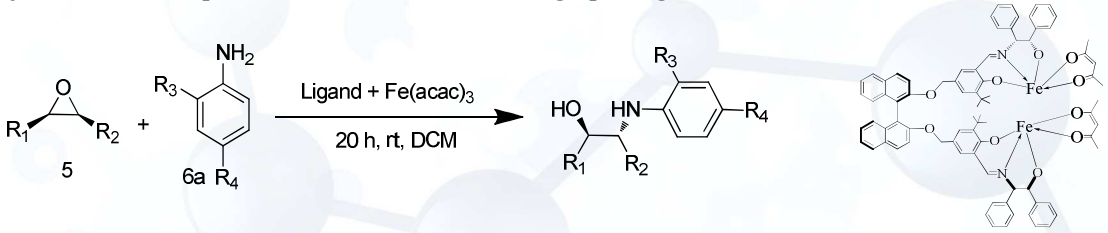
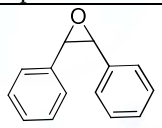
The desymmetrization of meso-epoxides by the anilines is a simple, precise and straight forward strategy for the synthesis of chiral β-amino alcohols.Chiral β-amino alcoholsare the class of compounds which finds its use in broad spectrum of applications in pharmaceuticals, agrochemicals, flavours, fragrances [1] and also as chiral auxilaries for asymmetric synthesis[2]. In literature diverse catalytic methods were reported for the synthesis of chiral β-amino alcohols among them the catalytic asymmetric ring opening (ARO) reaction of an epoxide with an amine is one of the best method [3], because it allows the formation of enantiopure β-amino alcohols in a single step with an atom efficiency. A number of efficient catalytic methods have been reported for the ARO of meso-epoxides with alkyl/aryl amines using catalysts based on chiral ligands with different metal ions *viz*., titanium,niobium, copper, lanthanides, chromium, iron, scandium, indium and bismuth to provide β-amino alcohols in excellent yield and enantioselectivity[4-5].But the recyclability of the chiral catalyst and enviromental issues with the reported catalyst motivated us to develop a efficient catalytic system for the ARO reaction. By keeping these issues in mind we have designed and synthesized a new chiral dinucleariron based catalyst which works efficiently in ARO reaction of meso-epoxide with aniline and it gives excellent yield (upto 95%) and enantioselectivity (upto 99%) of the chiral β-amino alcohols.

Keywords: Meso epoxides, Amino-Alcohols, ring opening



Entry	Epoxides	Anilines	Time	Yield (%)	*ee* (%)
1	 Stilbene oxide	Aniline	20	95	99
2		2-OMe	18	92	96
3		4-OMe	18	90	94
4		2-Cl	24	75	96
5		2-Me	22	86	89

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P-57

Enantioselective aza Henry reaction of isatin derived *N*-Boc ketimines By chiral Cu(II) macrocyclic salen complex

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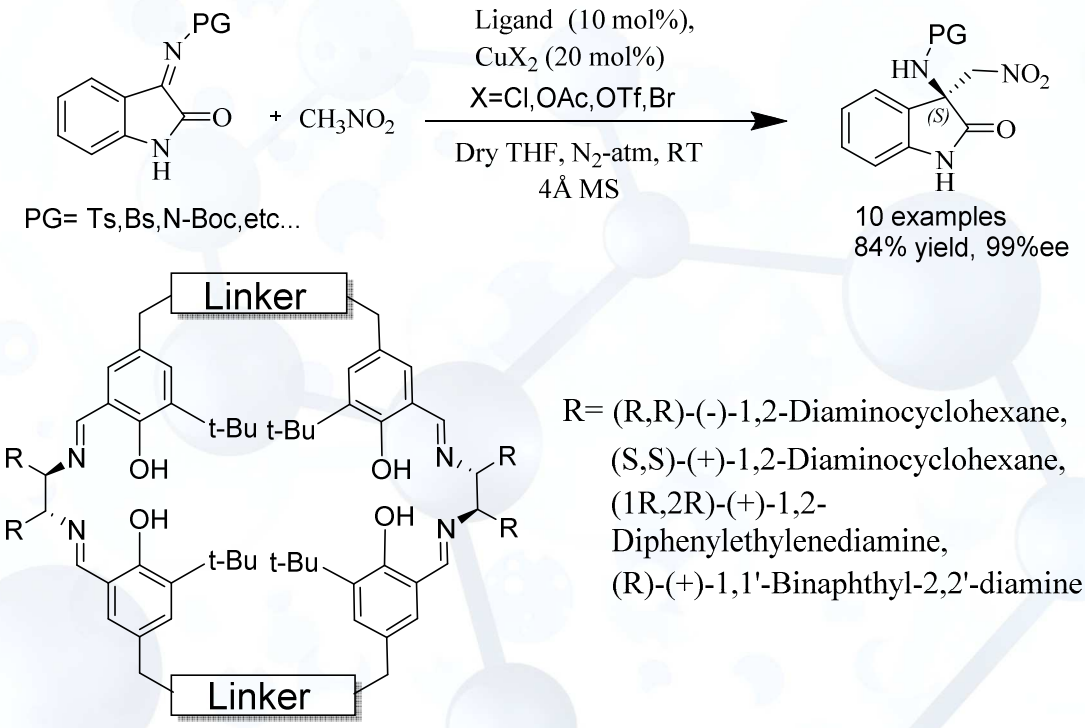
Recyclable chiral Cu(II) macrocyclic salen complex generated *in situ* efficiently catalyzed asymmetric aza Henry reaction of various isatin derived *N*-Boc ketimines with nitromethane as nucleophile at RT to give a high yield (88%) of β-nitro amines with excellent chiral induction (ee, up to 99%) with the added advantage of several times catalyst recyclability. This catalytic system also worked well with nitroethane and 1-nitropropane to furnish the corresponding products in high yields and enantioselectivties for *syn* diastereomers. Based on experimental observations a probable mechanism was proposed for this reaction. This protocol is also used for the synthesis of enantiomerically pure (*R*)-β-diamines via asymmetric aza Henry reaction of *N*-Boc ketimine in two steps in good yield with high enantioselectivity.

Keywords: Asymmetric aza Henry reaction; *N*-Boc ketimines; Cu(II) macrocyclic salen; β-diamines; recyclable



P-58

Development and validation of a Reversed-phase high performance liquid chromatography method for the Determination of 3-Methylbenzofuran-2-carboxylic acid and process related Impurities

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Abstract: A simple, selective, accurate and linear RP-HPLC method was developed and validation for the Determination of 3-Methylbenzofuran-2-carboxylic acid and process related Impurities accomplished in the bulk drug using a Reversed Phase High Performance liquid chromatography method with UV detection separation was achieved on Agilent SB C18 (250× 4.6 mm,3.5µm) as stationary phase with binary gradient mode solvent phase A. composed of 0.5 gm Ammonium acetate in1000ml water buffer (P^H adjust =3.5, with Acetic acid) and phase B of use filter & degas Acetonitrile ,The Flow rate of the mobile phase was 1.0 ml/min and the total elution time including the column re-equilibration was approximately 50 min. The UV detection wavelength was 254 nm ,Injection volume was 10µl and experiments were conducted at 40 °C temperature .The developed method was validated in terms of system suitability, selectivity, linearity, limits of detection and quantification the for the 3-Methylbenzofuran-2-carboxylic acid and process related Impurities.

Keyword: 3-Methylbenzofuran-2-carboxylic acid, process related Impurities, system suitability, binary gradient.

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STABILITY EVALUATION AND RAPID QUANTITATIVE DETERMINATION OF MILNACIPRAN BY UPLC METHOD

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Abstract: A method for stability study and rapid analysis required for quantification of Milancipran in pharmaceutical dosage form. A new rapid method developed using latest and fast chromatographic technique Ultra performance liquid chromatography (UPLC). Method developed on Aquity BEH C18 (100*2.11mm), 1.7µm column and 0.05% TFA in water as a mobile phase having a short runtime of 4 minute only. Method was validated as per ICH guideline and accuracy, precision, Linearity, robustness, LOD and LOQ study performed. Solution stability of milnacipran studied for 48 hrs. . Milnacipran was subjected to acid and alkali hydrolysis, chemical oxidation, heat degradation, and photo (sunlight) degradation. Method was optimised so that the degraded product peaks were well resolved from the drug signal with significant difference in their retention time value. A rapid method for quantitative analysis of Milnacipran was developed and method can be used for quantitative analysis in Quality control department.

Keywords: Milnacipran, Stability, UPLC, Validation

P-60

Mixed micelles and polymeric micelles as drug solubilizing agents and drug delivery vehicles.

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Abstract: A number of drug molecules are amphiphilic and henceform small aggregates by self-association in aqueous environment. Many pharmacologically active compounds are hydrophobicand cannot travel through the water based bodysystems. Amphiphilic drugs bear an ionic or nonionic polarheadgroup and a hydrophobic portion. They tend to self-associateas micelles in aqueous solution in a surfactantlikemanner. It is known that drug self-association depends on themolecular structure of the drug, the drug concentration,and physicochemical conditions such as temperature,pH, ionic strength, and additive concentration. Amphiphilic drugs solubilize in body fluids and interactwith membranes in the organism before they reach theirfinal targets. Aggregates of theseamphiphilic drugs could act as their own carriers. Mixed micelles and polymeric micelles havebeen extensively used as drug solubilizing agents as wellas drug delivery vehicles.Self-aggregationmechanism of amphiphilic drugs and their interactionswith surfactants in aqueous solution is of greatimportance in the rational design of more effective drug delivery systems.Over the years, therefore,micelles have been of interest to pharmacological scientistseither as drug delivery systems or as targeting systems.

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P-61

Visible-light-promoted difunctionylation of alkenes: an organophotoredox catalytic approach to β-keto sulfoxidation

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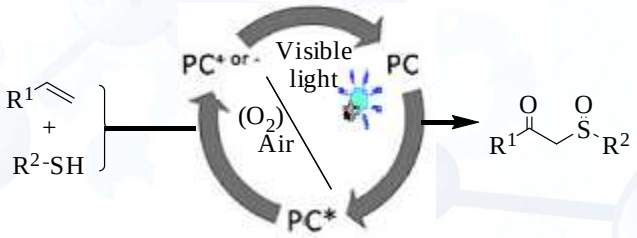
The ability of natural light (solar energy) for catalytic activation of organic molecules to achieve synthetically useful transformations has led to a flurry of activity in this area.[1-3] Consequently, visible light photoredox catalysis has recently emerged as a powerful means for the development of novel synthetic methodologies.[4] The success of this strategy has been mainly derived from the seminal work of the groups of MacMillan,[1] Yoon,[2] and Stephenson,[3] who employed $Ru(bpy)_3Cl_2$ (bpy = 2,2'-bipyridine) and $Ir(dtbbpy)_3Cl_2$ (dtbbpy = 4,4'-di-*tert*-butyl-2,2'-bipyridine) as the efficient photoredox catalysts. Although ruthenium and iridium transition metal complexes have proved to be efficient visible light photoredox catalysts, they suffer from disadvantages such as high cost, potential toxicity and low sustainability. The molecular oxygen in air has been broadly used as an environmentally benign oxidant in synthesis. In this context, we have developed a novel, metal-free and direct pathway for the difunctionalization of alkenes through photo-catalyzed oxidative sulfoxidation using eosin Y as an organocatalyst. The reaction involves thiophenol as a donor and O_2 as an acceptor to complete the catalytic cycle. Notably, it does not require any sacrificial donor or acceptor and hydrogen peroxide is the only byproduct of the reaction, which is also utilised *in situ* to oxidise sulfides to sulfoxides.



Scheme 1: Photo-catalyzed aerobic difunctionalization of alkenes

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

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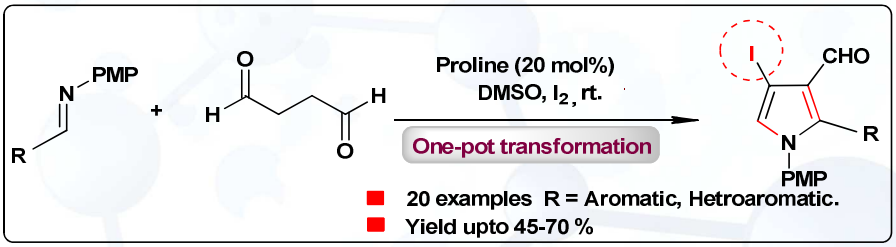
Abstract: The pyrrole nucleus is widespread in nature and the key structural fragment of heme(hemoglobin) and chlorophyll[1].Pyrrolemoietypresent in numerous biologically active natural products such as antiviral, anti-tumor, anti-oxidative, anti-inflammatory drugs[2]. Synthesis of pyrrole ring system has been attracted great attention of synthetic chemist in recent years[3].In continuation of our interest in organocatalyzed reactions, using linear dicarbonyl compounds as *donor-acceptor* precursors, recently, we developed an efficient organocatalytic method using succinaldehyde as 1, 3-carbon dipole and imines for the synthesis of 2,3- disubstituted pyrroles in high yields (upto 82%)[4]. The present idea of succinaldehyde as 1, 3- carbon dipole with imines through [3+2] annulation followed by via I_2mediated one pot oxidation protocol is very compatible and even more greener as compared to the methods known earlier[5]for the synthesis of 2, 3, 4-trisubstituted pyrroles from 1,4-dicarbonyl compounds(2, 3-disubstituted 4-iodo pyrroles).4-iodo pyrroles have been found asa useful synthetic substrates for the synthesis of biologically important heterocycles[6].Organocatalytic[3+2] annulation of succinaldehyde with imines followed by I_2 mediate oxidation for the regioselective synthesis of 2, 3-disubstituted 4-iodo pyrroles in one pot will be presented here.This method can be further utilized for the synthesis of some small molecule natural products. (**Scheme 1**).



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

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P-63

Synthesis of Bis(2-arylimidazo[1,2-*a*]pyridin-3-yl)methane*using* $VO(acac)_2$/IBD Catalyzed Reaction of Imidazo[1,2-*a*]pyridine with Diemethylacetamide

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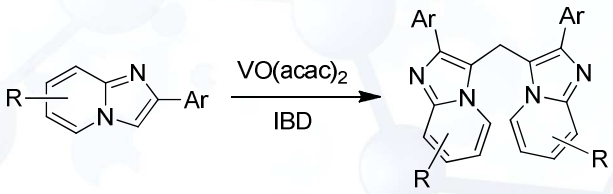
Bis(heteroaryl)methanes have attracted attention of chemists in recent years owing to their wide spectrum of biological activities.[1]Several reports are available on synthesis of bis(indolyl)methanes using aldehydes[2] and derived aldehydes[1a] as methylene linkage but very few reports are available for other bis(heteroaryl)methanes including that of imidazo[1,2-*a*]pyridines.[3] Imidazo[1,2-*a*]pyridine skeleton has been found to exhibit several biological activities such as antiviral, antibacterial, antifungal, ATPase inhibition, anti-rhinoviral, antiulcer and antihelminthics. They are also core structure of many marketed drugs such as alpidem, zolpidem and saripidem. In these drug molecules methylene linkage is present at C-3 position.[4]

Recently, our group has been involved in developing new methods of functionalization of imidazo[1,2-*a*]pyridines,[5] in this poster we will present our initial results for synthesis of bis(2-arylimidazo[1,2-*a*]pyridin-3-yl)methane using$VO(acac)_2$ catalyzed reaction of imidazo[1,2-*a*]pyridine with diemethylacetamide in the presence of iodobenzene diacetate (IBD) as oxidant (Scheme 1). The reaction involves coupling of sp^3-sp^2 carbons and proceeds through formation of iminium ion. A wide variety of imidazo[1,2-*a*]pyridines resulted corresponding bis(imidazo[1,2-*a*]pyridin-3-yl)methanes in good to excellent yields. A gram-scale reaction demonstrated the potential for the scale-up processes.



Scheme 1: Synthesis of bis(2-arylimidazo[1,2-a]pyridin-3-yl)methanes

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P-64

Synthesis and Biological Evaluation of Novel Carbazolyl Glyoxamides as Anticancer and Antibacterial Agents

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Indole alkaloids are widely present in numerous natural products and synthetic molecules which are of immense biological importance in organic and medicinal chemistry [1]. Particularly, tricyclic heteroaromatic indole alkaloids such as carbazoles are an important class of natural and synthetic organic compounds. In the last few decades medicinal roles of natural as well as synthetic carbazoles have expanded significantly, especially as a vital heterocyclic class of antitumor and antibacterial agents [2]. Naturally occurring carbazoles, for example, ellipticine, olivacine, granulatimide and carbazomycins etc. have displayed significant anticancer and antibacterial activities [3]. On the other hand, glyoxamide is an useful motif widely present in many biologically active compounds and synthetic drug candidates, especially, indolylglyoxyamides like indibulin, coscinamides and bis(indole)glyoxamides endowed with interesting anticancer and antibacterial properties [4]. In our continuous efforts to identify indole-based bioactive molecules, we prepared α-cyano bis(indolyl) chalcones, 2-arylamino-5-(3′-indolyl)-1,3,4-oxadiazoles, 2-arylamino-5-(3′-indolyl)-1,3,4-thiadiazoles, indolyl-1,2,4-triazoles as potent anticancer agents. Very recently, we have identified 2-(3′-indolyl)-*N*-arylthiazole-4-carboxamides as potent anticancer and antibacterial agents [5]. Encouraged by the promising biological activities of glyoxamides and pivotal roles of carbazole scaffold in bioactive compounds prompted us to investigate their new analogues. We have designed carbazolyl glyoxamides by incorporating important scaffolds, glyoxamide and carbazole in a single molecule. A library of carbazolyl glyoxamides was prepared from carbazole glyoxalic acids and arylamines in presence of HATU as a coupling reagent under MW irradiation. Some of the synthesized carbazolyl glyoxamides were found to exhibit interesting *in-vitro* anticancer activity with IC_{50} values in low micromolar range against a panel of cancer cell lines and displayed exciting antibacterial activity against tested bacterial strains. Synthesis, characterization, biological activities of the newly prepared carbazolyl glyoxamides will be discussed in the poster presentation.

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P-65

Microwave-Assisted Metal and Ligand-Free O-Arylation of Quinolones Using Diaryliodonium Salts

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Quinolines are key building blocks of many interesting bioactive molecules [1]. Many compounds with this nucleus have been found to display various biological activity including antimalarial, antimicrobial, antiasthmatic, antituberculosis, antileishmanial, anti-HIV, and anticancer [2]. Owing to these important medicinal properties, there is a growing interest to functionalize the quinoline scaffold to make 'drug-like' small molecules for biological screening. Recently, C-2 and C-4 positions of quinoline heterocycles have been modified by introducing a number of carbon, oxygen, nitrogen and sulphur-based nucleophiles to achieve substituted quinolines. Quinolin-2(1*H*)-ones and quinolin-4(1*H*)-ones are the crucial precursors for the preparation of quinolylarylethers which are endowed with interesting biological profile [3]. In recent years, diaryliodonium salts have received much attention as powerful electrophilic arylating agents due to their high reactivity, stability and low toxicity. They have been employed in a variety of metal-free as well as in metal-catalyzed arylation reactions leading to the formation of biologically important heterocycles [4]. Most of the arylation reaction involved transition-metal catalyst and ligands which are normally very expensive, air-sensitive, toxic to different extents and their removal from the desired products is laborious and challenging in medicinal chemistry research. Our continuous efforts to explore the synthetic utility of diaryliodonium salts as arylating agents [5] and in view of potential pharmacological properties associated with aryloxyquinolines, we wish to report a novel metal-free direct O-arylation of quinolones utilizing readily available and stable diaryliodonium salts to access a diverse series of aryloxyquinolines. Optimization of the reaction conditions, substrate scopes, mechanism and characterizations will be presented in conference.

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P-66

Enantioselective copper-catalyzed direct C-N/C-O coupling in water: A facile access to fluorescent labelled amino acids and *Leu-enkephalin*

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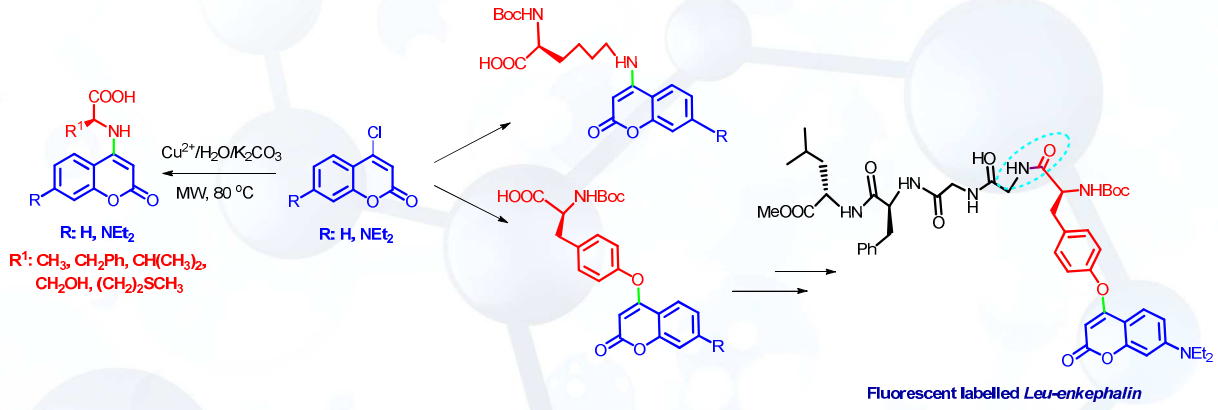
Site specific labelling of amino acids and peptides with a fluorescent probe or inclusion of a fluorescent labelled amino acid at definite sites in protein are excellent strategies used for studying *in vitro* and *in vivo* biological processes such as receptor-ligand binding and protein-protein interactions *via* labelling studies.[1]Continued research for extracting the exact mechanism of the above ubiquitous biological processes using labelling studies and limitations in the existing synthetic strategies has opened doors for the development of newer synthetic methodologies for integrating fluorescent scaffolds into amino acid, peptides and proteins.

In recent years, microwave heating in combination with water has become an ally of choice for swifting the rate of cross-coupling reactions, for the formation of C-N and C-O bonds in a clean and greener way. Copper catalyzed arylationreactions devoted to the formation of C-heteroatom bonds (Ullmann type coupling) have been broadly acknowledged[2] due to its applicability to perform reactions under environmental benign condition.[3]As a part of our continuing interest in synthesizing novel fluorescent amino acids,[4]we herein report a mild, efficient and greener methodology for the enantioselective synthesis of coumaryl labelled amino acids through microwave-assisted copper-catalyzed direct C-N coupling in water. The photo-physical properties of the synthesized compounds have been studied. The methodology was extended for direct C-O and C-N coupling in water to yield fluorescent side chain functionalized coumaryl labelled tyrosine and lysine derivatives respectively. In addition, chemical application of coumaryl labelled tyrosine was investigated towards the synthesis of fluorescent opioid pentapeptide neurotransmitter, Leu-Enkephalin.



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P-67

Synthesis, Characterization of Schiff bases with transition metals and its remarkable study of human anti-breast cancer cell lines

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Abstract: Schiff bases play an important role as ligands in metal coordination chemistry even after almost a century since their discovery. Modern chemists still prepare Schiff base ligands are considered as "privileged ligands" They were also reported to possess, cytotoxicity[1], anticonvulsant[2], anticancer[3], and catalysis[5],

A series of novel compounds whose structures are Schiff base based skeleton have been synthesized and characterized. These Schiff bases were derived from aryl aldehydes and 5-(3-Bromo-4-methoxyphenyl)-4-{[substitutedphenylmethylidene]amino}-4H-1,2,4-triazole-3-thiol. Most of the reactions have been successfully applied and used, as many of the synthesized compounds exhibit interesting biological activity in the fields. The structures of synthesized compounds were established on the basis of ^{1}H NMR, FTIR spectroscopy as well as by X-ray diffraction. The compounds were evaluated for in vitro anticancer activity.The most active compounds from the series displayed GI50 value equal to doxorubicin against the strain of human breast cancer cell line MCF-7.

Keywords: Schiff bases, transition metal, anti-cancer activity.

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Enantioselective synthesis of 1,2-dihydropyridines via formal [4+2] cycloaddition between aqueous glutaraldehyde and imines

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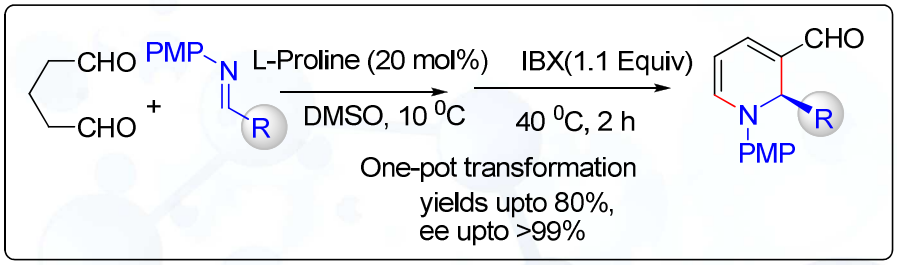
Dihydropyridines are pyridine ring based organic scaffolds encountered in nature and possessing broad andmany interesting biological activities **[1].** In particular, 1,2-dihydropyridines(DHPs)are important building blocks to synthesize awide range of organic molecule, such as piperidines, pyridines, quinolizidine skeletons.**[2]** 1,2-DHPs found in many synthetic compounds and also being considered as suitable cyclic aza-dienes for Diels-Alder reaction to prepare isoquinuclidines**[3],** an important structural motifs for the variety of natural products **[4].** Owing to their high synthetic and biological importance, efforts have been directed towards the synthesis of 1,2-DHPs. Synthetic efforts for the 1,2-DHP skeleton can be broadly divided into two main categories; *(i) Nucleophilic addition to activated pyridines***[5]**and*(ii) 6π-electrocyclization of 1-azatrienes***[6].**These two synthetic approaches along with others have recently been reviewed **[7].** Asymmetric synthesis of 1,2-DHPs remains a challenging task and almost untouched except few efforts **[8].** Organocatalyticone pot enantioselective synthesis of 1,2-DHPs will be presented here.



Scheme 1: Organocatalytic [4+2] annulation/IBX oxidation sequence for the synthesis of 1,2 dihydropyridines

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P-69

Hybrid approach towards the synthesis of natural product inspire novel Quinoline - imidazolone based scaffolds as potential anti-parasitic agents

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Abstract: At the border between bio-inspired and rational drug design, one can imagine preparation of hybrid molecules with a dual mode of action to create efficient new drugs. Hybrid molecules are defined as chemical entities with two or more structural domains having different biological functions and dual activity.[1] Aplysinopsin has recently been discovered as a potential antimalarial agent.[2] In the continuation of our ongoing programme to develop new hybrid molecules as potent anti-parasitic agents,[3] and inspired by the antileishmanial and antimalarial activity of Quinoline and imidazolone based natural product chloroquine and Aplysinopsin, we herein report our work on the design, synthesis and anti-protozoal evaluation of novel Quinoline - imidazolone hybrids (Fig. 1)

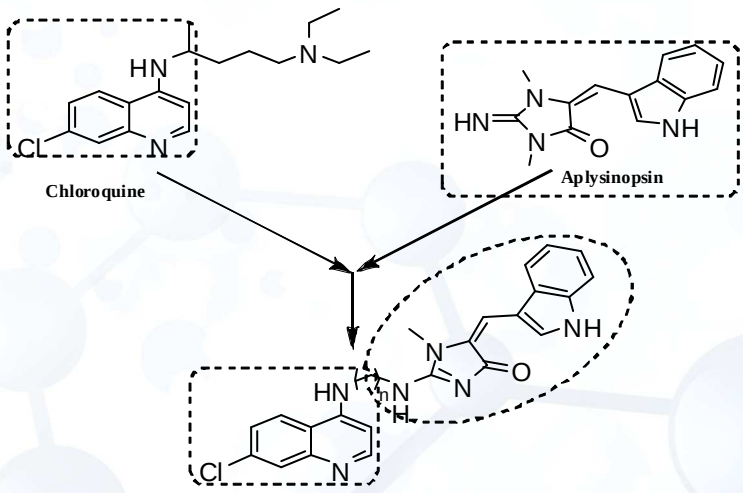

Fig. 1: Chloroquine-Aplysinopsin Hybrid

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An Efficient Synthesis of highly functionalized Dihydrooxazinone*via*Copper- Mediated IntramolecularDehydrogenative Coupling of Ugiadduct

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The Ugi four-component reaction (Ugi-4CR)[1]is one of the highly investigated multicomponent reaction for generating multifunctional adducts, owing to the mildness of the reaction conditions, the wide application scope and the high variability (four diversity points) associated with it. Moreover, it provides an opportunity for a numerous of post-transformations depending on the functional groups introduced during the MCR, thus leading to the synthesis of several pharmacologically important heterocyclic scaffolds, mostly in two operational steps[2].The dihydro-oxazinone moiety is found in a number of pharmaceutically relevant scaffolds such as CX-614[3] and DRF-2519[4].In the past few years, we have been involved in the multicomponent Ugi reactions and post-ugi transformations for generation of natural product-like compounds[5].In this context, we planned to study copper-Mediated synthesis of Dihydrooxazinone through regioselective C-H bondactivation and cyclization of Ugi precursor. This post-ugi transformation gave opportunity to synthesis divers highly functionalized Dihydrooxazinone.

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P-71

Discovery of Small Molecules for the Protection of Obesity induced Memory impairment via bio-screening cascade

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Current facts show an association between obesity and cognitive decline[1]. In present study we have synthesized lactum library *via* ugi 4CC reaction and study their effects in biological screening cascade. Compound-5h emerged out as most active entity in screening cascade assay that considerably inhibit the HMG-CoAR activity in vitro, lipids concentration in triton-WR 1339 induced hyperlipidemic rats and amyliod beta (Aβ)[2] deposition in caenorhabditis elegans followed by decrease in lipids and oxidative stress. Consequently, docking model for HMG-CoAR inhibition was developed which explore the possible binding modes of compound-5h to receptors HMG-CoAR cavity at molecular level. Therefore, we considered a lead molecule compound-5h might be a potential treatment to ameliorate age-related decline in cognitive function, particularly on obesity induced dyslipidemia environment, where improvements in circulatory cholesterol which enters in central nervous system (CNS) through blood brain barrier (BBB) which may facilitate recovery of cognitive function[3]. Hence we developed an animal model to examine the amelioration potential of compound-5h for combined obesity and neurocognitive deficits resulting from two months high-fat diet feeding in middle-age rats. Considerably one month chronic treatment of compound-5h reduced gain in body weight and improves dyslipidemic factors. Behaviorally, it enhanced gaining of learning in Morris water maze test, this phenomenon reduced inflammation, oxidative stress and alteration in brain amyloid precursor protein (APP), beta secretase (BACE), Glial fibrillary acidic protein (GFAP), tau phosphorylation (P-tau) and apoptosis signalling pathway which can play a pivotal role in the early onset of memory loss[4][5]. Eventually compound 5h was showing protection of obesity induced memory impairment by regulating the HMG-CoAR activity in both liver and brain. Taken together, these results suggest that compound-5h modulates hippocampal and cortex circuitry effectively to promote an improvement in cognitive function.

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P-72

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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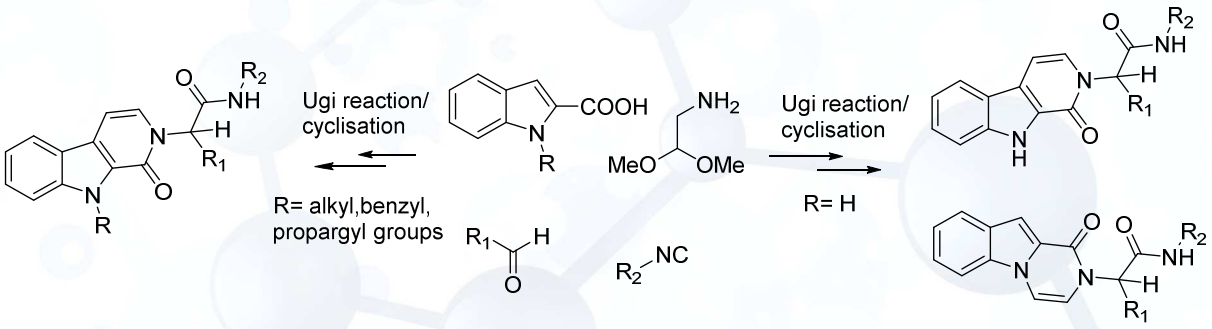
Abstract: Indole heterocyclic, ß-carboline core containing natural products and related synthetic derivatives have found extensive application in medicinal chemistry as antitumour, antimalarial, antileishmanial, anticancer, and other life style related diseases [1]. A number of clinical therapeutics such as indomethacin, indoramin, and indorenate also consist of an indole moiety. Indole nucleus containing natural product such as ß-carboline, ß-carbolinone, spirooxindolesetc, are not limited to privileged structures that have the ability to bind with several receptors else the attractive scaffolds for drug discovery [2].

In the light of above fact, herein we report an efficient one pot two step process for the synthesis of *β*-carbolinone and Indolo-pyrazinoneanalogushas been developed. This protocol involves the Ugi four-component reaction (U-4CR) followed by an intramolecularacid-mediated deprotection/activation/electrophilic cyclisation/and aromatisation of the Ugi products at room temperature(35 ºC) to afford the desired products in good to excellent yields. In addition, we synthesized N-substituted *β*-carbolinonesheterocycles of medicinal importance using N-substituted derivatives of indole 2-carboxy acid.



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P-73

Metal-Free Isocyanide Insertion Reaction with Amines: A Divergent Synthesis of Ureas

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Isocyanides have widely established themselves to be unique building blocks in modern organic chemistry[1]. The extraordinary features of the isocyano group make isocyanides particularly useful for the synthesis of a number of important classes of nitrogen heterocycles, such as pyrroles, indoles, and quinolines. Several cocyclizations of isocyanides *via* zwitterions and radical intermediates as well as transition-metalcatalyzed syntheses of different types of heterocycles have recently been developed[2].An I_2/TBHP-mediated cross-coupling reaction of isocyanides with readily accessible amines *via* C−N formation is described for Urea synthesis in moderate to excellent yields. This represents a metal-free strategy for a coupling reaction of isocyanides with amines, and it provides an efficient approach for symmetric and unsymmetric functionalized Urea derivative synthesis under mild conditions.

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P-74

Biological activities of newly synthesized benzothiazole based analogs.

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Abstract: Benzothiazole have received considerable attention because of their interesting pharmacological activities including anticonvulsant [1], analgesic [2] anti-tumor [3,4] antibacterial [5,6], antimicrobial [7,8] and muscle relaxant agents.[9] As an aspect of our ongoing research in search of new antimicrobial armamentarium, a series of benzothiazole based acetamide, pyrazole and Pyrrole were synthesized and analyzed for their *in vitro* antimicrobial activity against several bacteria, fungi, and some of the selected compounds were also tested for their antitubercular activity. The structural assignments of the all analogs were done on the basis of IR, ^{1}H NMR, Mass spectroscopy and elemental analysis. The biological screening identified that some compounds showed better or similar activity compared to reference drugs. A structure-activity relationship study was explored to facilitate further development of this new class of compounds. Interestingly, it was noticed that the potency of final analogs against each strain placed reliance on the type of moiety (acetamide, pyrazole and pyrrole) present on benzothiazole.

Keywords: Benzothiazole, Antifungal, Antibacterial, Antitubercular activity

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P-75

Organocatalytic synthesis of *N*-aryl substituted pyrrolo-pyridazinones from ethylglyoxalate, *p*-anisidine and succinaldehyde and various hydrazines

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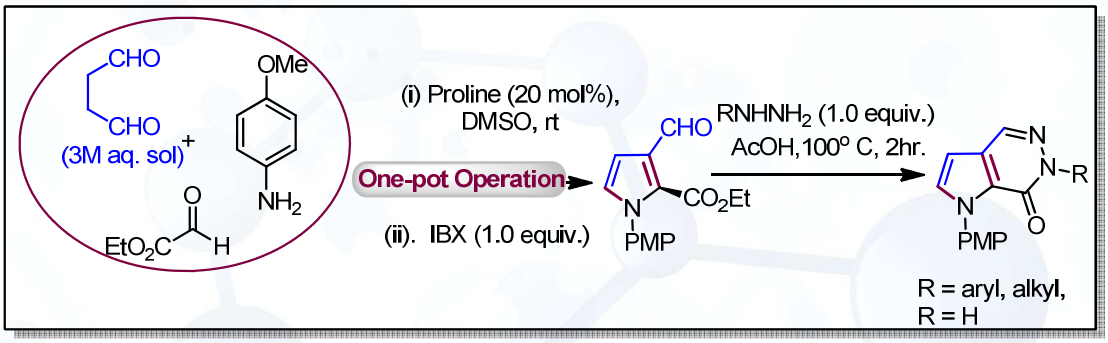
Pyridazinones and their *N*-aryl substituted derivatives are building blocks for many biologically active compounds such as pharmaceuticals, pesticides,and also found to have potential antibacterial, antifungal, antiviral including anti-HIV activities, anticancer, analgesic & anti-inflammatory, anticonvulsant activities.[1] Based on our previous reported work using linear dicarbonyl compoundssuch as succinaldehyde which acts as as donor-acceptor (D-A) precursor for the direct synthesis of di-substituted and densely substituted-3-formylpyrroles with formyl functionality at C3 position under mild conditions in high yields,[2] which in turn is an alternative to Paal-Knorr strategy.[3] Presently we establishednew and quick strategy for the synthesis of *N*-aryl substituted pyrrolo-pyridazinones through direct Mannich annulation of ethylglyoxalate,*p*-anisidine, succinaldehyde and various substituted hydrazines. It was found that the use of proline as an organocatalysts achieves highly efficient C−C and C-N bond formation and in situ aromatization using IBX as mild oxidizing agent, further followed by condensation and complete cyclization with different hydrazines *via* multi-component one-pot sequential approach in just two steps. Details of this work will be presented here (**Scheme 1**).



Scheme 1: Organocatalyzed one-pot multi-component synthesis of *N*-aryl-pyrrolo [2, 3-d] pyridazin-7(6H)-one

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P-76

Sugar-based Novel Chiral Macrocycles for Inclusion Applications and Chiral Recognition

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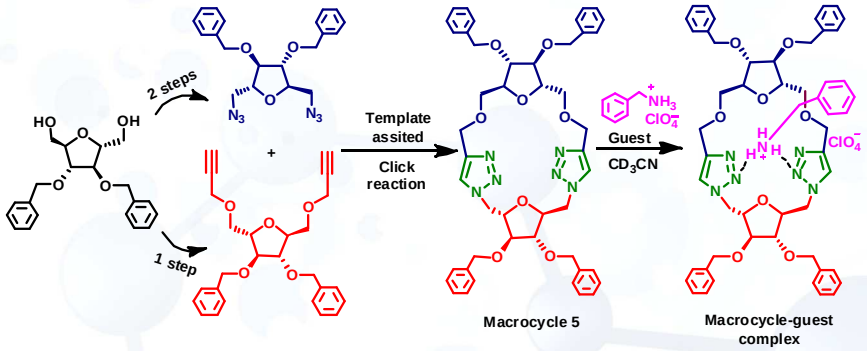
Macrocycles have diverse applications as molecular pores, biomimetic receptors and chiral recognition agents. We have successfully accomplished a highly convergent synthesis of chiral macrocycles which are cyclic homodimer of azido-alkyne pentose sugar derived from 2,5 anhydro-D-mannitol. It has been observed that the addition of template and high dilution factor of the reaction enhance the % yields. Further, the host guest inclusion studies have also been performed by using benzyl ammonium perchlorate salt as guest. The studies revealed a significant interaction between the host macrocycle and the guest primary ammonium salt over secondary ammonium salt, as observed through various spectroscopic techniques. The synthesised macrocycle also shows chiral recognition ability with *L*-phenylalanine hydrochloride methyl ester over *D*-phenylalanine hydrochloride methyl ester, further that has been confirmed by molecular modelling studies. The detailed synthetic schemes and interaction studies will be discussed during the poster presentation.



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Synthesis, Thermal behavior and antimicrobial activity of polyester based on 5-(3,5-dinitrobenzoylamino) Isophthalic Acid

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Abstract: Novel aromatic polyesters having pendent group based on 5-(3,5-dinitrobenzoylamino) Isophthalic Acid have been synthesized with moderate molecular weights by phase transfer catalyst (PTC) method. Prepared polyesters were characterized by FT-IR, Thermogravametric method and GPC. Polyersters are soluble in polar solvent. DSC and TGA data indicates that polyesters are thermally stable. Antimicrobial activity of the polyesters shows that they inhibit the growth of microorganisms to considerable extent**.**

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Synthesis, characterization and application of polyether based on 4,7-Dichlro-6-Nitroquinazoline

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Abstract: Novel hetrocyclic polyethers containing 4,7-Dichlro-6-Nitroquinazoline have been synthesized with moderate molecular weights by direct polycondensation method. The polyethers were characterized by FT-IR, H1-NMR, DSC, TGA and GPC. Solubility data of polyethers exhibit good solubility in polar solvents. Thermogravametric data showed that these polyethers are thermally stable. Antimicrobial activity of the polyethers indicates that they inhibit the growth of microorganisms**.**

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Food restriction reduces obesity but does not improve Leptin gene expression in WNIN/Obese rats

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Background/Objectives: Leptin an adipokine, deregulated in many cases of obesity is poorly understood undernutrition interventional strategies like food restriction. The present study addresses the aboveusing a genetically obese rat strain, WNIN/Ob.

Subjects/Methods: Lean and Obese rats of WNIN/Ob, aged 35 days were allotted to three groups: (1) Lean_Ad(fed *ad libitum)*, (2) Obese_Ad (fed *ad libitum)*, and (3) Obese_Fr (under 60%foodrestriction), with 4 animals per group (n=4). Rats were fed up to 90 days age, after which they were assessed for physical and biochemical parameters. Statistics; Mean, Standard Error, 95%CI of Mean and fold differences of mean were used to describe the data. Differences between groups was inferred for statistical significance by Independent samples T test with $p<0.05$.

Results: Obese_Ad rats in comparison with Lean_Ad showed significantly higher body weights (501-637 vs 256-330 in grams), fat percentages (54.8-55.8 vs 13.3-17.1), circulating triglycerides(192.2±20 vs 99.2±17.7 in mg/dl), TBARS (11.8±0.5 vs 4.8±0.2 in nmol/ml), and Leptin(43.2±6.4 vs 0.58±0.0 in ng/dl). Food restriction in obese rats (Obese_Fr) has reversed allthe above parameters to that of Lean_Ad rats except for Leptin. Circulating Leptin Levels inObese_Fr rats (25.36±2.3 ng/dL) though significantly reduced compared to obese_Ad rats,this reduction was negligible with respect to Lean_Ad rats. Leptin gene expression in whiteadipose tissue (4.49 and 4.0 fold increase in Obese_Ad and obese_Fr rats with respect toLean_Ad rats) supports the above observation.

Conclusions: Food restriction, normally known to reduce Leptin expression, its regulation is impaired inobese rats of WNIN/Ob. Results suggest that mere food restriction may not ameliorate all thefacets of metabolic syndrome and may not be a safer practice. Further studies are required toaddress this impaired mechanism.

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SYNTHESIS AND CHARACTERIZATION OF NOVEL SUBSTITUTED 4'-{4-[1-ACETYL-5-(4-CHLORO-PHENYL)-4,5-DIHYDRO-1H-PYRAZOL-3-YL]-PHENOXYMETHYL}-BIPHENYL-2-CARBONITRILE

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Abstract: Pyrazoline derivatives are well renowned for having valuable pharmacological properties. In the present work, series of diversely substituted Pyrazoline functionalized with Biphenyl carbonitrile moieties have been synthesized. The reaction of 4'-Bromomethyl-biphenyl-2-carbonitrile with 1-(4-Hydroxy-phenyl)-ethanone resulted 4'-(4-Acetyl-phenoxymethyl)-biphenyl-2-carbonitrile **(AC-1).** AC-1 was subjected to Claisen-Schmidt condensation with substituted aromatic aldehyde in mixed solvent afforded various substituted 4'-[4-(3-Phenyl-acryloyl)-phenoxymethyl]-biphenyl-2-carbonitrile **(AC-2)** which is commonly known as Chalcones. Chalcones were further cyclized with Hydrazine hydrate in presence of glacial Acetic acid to produce 4'-{4-[1-Acetyl-5-(4-chloro-phenyl)-4,5-dihydro-1H-pyrazol-3-yl]-phenoxymethyl}-biphenyl-2-carbonitrile **(APC, A-L).** The chemical structures of synthesized compounds were characterized by ^{1}H-NMR, ^{13}C-NMR and FT-IR. Synthesized compounds were screened for their antimicrobial activity by Broth dilution method.

Keywords: Pyrazoline, Antimicrobial, Antifungal.

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Hair growth potential of an Extract from *Trichosanthes dioica*

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Trichosanthes dioica Roxb. (family: Cucurbitaceae), commonly known as "Sespadula" in English and "Parwal" in Hindi, is widely grown throughout India. It possesses anthelminitic, antihyperglycaemic, antioxidant, antidiabetic, antipyretic, cholesterol-lowering hepatoprotective and wound healing activity. The leaves of this plant are topically used to promote hair growth in traditional ayurvedic preparations. The chopped leaves of *Trichosanthes dioica* was extracted with acetone. We have separated fat from this extract using acetonitrile. The fat free extract showed significant 5- α reductase inhibitory activity. The phytochemical examination of this extract is in progress.

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Antidandruff activity of *Buchnania lanzan* seeds

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Buchnania lanzan Spreng syn. *B. latifolia* Roxb. known locally as char, piyal, achar or chironji belongs to the family Anacardiaceae. The seeds of Buchnania lanzan are used as astringent, general and cardio tonic as well as for curing skin diseases and removing spots/blemishes from the face. The paste of seeds is applied on hair to control dandruff. The oil extracted from kernels known as "char" is used in some antidandruff ayurvedic formulations. We have obtained viscous oil from petroleum ether extracts of seeds and separated fats from this oil using acetonitrile. The GC-MS analysis of this fat and its antidandruff activity is under progress.

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Distinct Blue Print to Restraint Neglected Tropical Diseases

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Abstract: Since, few decades many developing countries are bearing the strain of Neglected Tropical Diseases (NTDs) and they are the most common infections of the World's poorest people living in Africa, Asia and Americas. Till date, neglected tropical diseases imitate a group of conditions whose cluster level is obtained from deficiency of efforts directed to their declination. Global efforts have been done to control thirteen parasitic and bacterial infections that affect more than 1.4 billion people. The global usage of drug therapies for reducing the severity of NTDs was introduced few years ago. This singular approach should be elaborate to more extensive set of tools like coordinated community-based programs, vector control, local training, education and environmental change. In more, accelerated schedule is crucially needed to establish adequate diagnostic, preventive and therapeutic interventions to stay one step ahead of the evolutionary adaptation system of disease-causing microorganisms and parasites.

Keywords: Neglected Tropical Diseases, Parasite, Microorganisms, Drug Therapy.

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P-84

SYNTHESIS AND CHARACTERIZATION OF TETRALONE BEARING NOVEL IMIDAZOLO AND TRIAZOLO-QUINAZOLINE DERIVATIVES

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The year 1891 was milestone for the finding a new class of chemist Pietro Biginelli**,** who first reported the simple one pot process that furnish organic compound of Biginelli adduct, also known as 3-4-dihydropyrimidine-2(1H)-ones/thiones (DHPMs) involves one pot reaction of three key building blocks, 1,3-dicarbonyl compounds, aldehydes and thiourea. Variation of three building blocks has broadened the molecular diversity of DHPMs with wide variety of biological activities. On the other hand, the importance of 1,2,4-triazole and quinazoline nuclei is well established in the field of organic and medicinal chemistry. In the view of important biological properties associated with triazoles and quinazoline, its worthwhile to incorporate both of these scaffolds in a single molecular framework for further evaluation of their biological profile.[1][2][3] To achieve this goal, we have synthesized a series of triazolo-quinazoline derivatives using tetralone and aldehyde as precursor in basic condition. The details study will be presented in the poster.

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ANTIMICROBIAL STUDIES OF 1-{2,4-DIMETHYL-5-[(5-SUBSTITUTEDPHENYL-1,3,4-OXADIAZOL-2-YL)CARBONYL]-1H-PYRROL-3-YL}ETHANONES BY AGAR DILUTION METHOD

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We live on the planet earth. The surroundings around us make our environment. The environment is made up of many live and dead things which are detrimental to our growth, development and sustenance. We try to save or improve it by many efforts in discussion as well as in implementation. Many microorganisms are deadly to human health. Especially when immune system of the person is weak or he suffers from killing diseases like AIDS. The commansals also become opportunists and causing serious complications in human body. We need to find medicine to cure the newly emerging multidrug resistant varieties of microbes. Bactericidal and fungicidal activities were reported for exazolidane, amino oxazodiozole, and oxadiazoline thiones (Desai, 2007).The tin derivatives in an effective fungicide and antimicrobial are shown by thiones. The oxazdidones have shown herbicidal and insecticidal activity (Upadhyay, 2006). For such a reason, a few chemists have synthesized several ethanones which were used to investigate their antimicrobial activity against several bacterial strains during primary, secondary and tertiary screening of the organic compounds with MIC using Agar Dilution Method recommended by NCCLs. surprisingly hopeful results were obtained which has proven the potential of the series to affect bacterial growth to certain considerable extent.

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ISOLATION AND CHARACTERIZATION OF PHYTOSTEROLS FROM *CORDIA MACLEODII* (HOOK F. AND THOMSON) BARK BY CHROMATOGRAPHIC AND SPECTROSCOPIC METHOD

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Aims and objectives: The study focuses on isolation and determination of the chemical constituents of the Cordia macleodii bark, used as medicinal plant in folklore system. The principle theme of the study is to develop applied chromatographic techniques for the separation, isolation and detection of the compounds.

Methods: A petroleum extract of bark were analyzed by GC/MS, IR, and UV. The structures were elucidated on the basis GC-MS library of reported data.

Result: Three known compounds Stigmasterol, Cholest-5-EN -3OL (3 Beta)-Carbonyl chlorinated, Camphesterol were determined from Cordia macleodii bark. These compounds were isolated from this plant for the first time.

Conclusion: From the present study, it is concluded that chromatographic and spectroscopy has potential as rapid and simple tools in the isolation and analysis of various compounds from Cordia macleodii bark.

Keywords: Gas chromatography-mass spectrometry, Infrared, Chromatography, Spectroscopy, Phytosterols, *Cordia macleodii*.

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SYNTHESIS AND CHARACTERIZATION OF SOME NOVEL THIAZOLE DERIVATIVES

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A series of substituted thiazole derivatives were synthesized by reaction of thiosemicarbazide with substituted vanillin under acidic condition and methanol as a solvent followed by cyclization using substituted phenacylbromides at room temperature.[1][2][3][4] The characterizations of synthesized compounds were done by ^{1}H and ^{13}C NMR and Mass spectroscopy.

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QUANTITATIVE ANALYSIS OF ANTIPLATELET DRUG TICAGRELOR IN BULK AND PHARMACEUTICAL DOSAGE FORM BY VALIDATED UV-SPECTROSCOPIC METHOD USING GREEN APPROACH

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Abstract: Ticagrelor is a platelet aggregation inhibitor drug, recently launched by Astra Zeneca as Brilinta. A rapid, specific and cost effective UV spectrophotometric method has been developed for the estimation of Ticagrelor in bulk and pharmaceutical dosage formulations.The optimum conditions for the analysis of the drug were established. The Ticagrelor content was determined using a greener solvent composed of 57:43 v/v methanol:water. Maximum absorption found to be at λ_{max} 222 nm. The method was validated based on ICH guidelines with respect to specificity, precision, linearity and accuracy. The analysis data has been subjected to statistical analysis and the results of this study are validated. Beers law was obeyed in the concentration range of 8- 32µg/ml having linear equation of Y = 0.0946 x + 0.0239.The percentage recovery of Ticagrelor is between 97.08 to 98.07%. The method developed is simple, sensitive, reliable and results are reproducible, hence useful for the routine analysis of Ticagrelor.

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HIGHLY EFFICIENT AND ECO-FRIENDLY ONE-POT SYNTHESIS OF PENTA SUBSTITUTE PYRROLE DERIVATIVES UNDER CATALYST-FREE CONDITIONS

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An eco-friendly and efficient one-pot synthesis of penta-substituted pyrrole derivatives via a four-component reaction of maldrum's acid, arylglyoxal monohydrate, dimethyl but-2-yne-dioate and amines under catalyst-free conditions in an environmentally friendly medium is described.[1][2] The simple experimental procedure, catalyst-free reaction conditions, short period of conversion, and excellent yields are the advantages of the present method. Good chemical yields have been achieved without the need for chromatography and recrystallization or other purification methods.[3][4][5]

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HIGH THROUGHPUT SIMULTANEOUS SCREENING OF SIX ANTIPSYCHOTIC MOLECULES BY UPLC

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Abstract: Antipsychotics are a class of psychiatric medication that are mainly used to treat mental health illnesses or used to manage psychosis such as schizophrenia, bipolar disorder[1][2][3][4]. Here some diverse antipsychotic molecules such as Amisulpride, Risperidone, Paliperidone, Aripiprazole, Ziprasidone and Lurasidone are taken into consideration for their simultaneous determination. The chromatographic separation was carried out by using Acquity UPLC@BEH shield RP C18 (100mm X 2.1mm id, 1.7µm particle size) column with 45°C column oven temperature. The detection was monitored at 242nm wavelength with 0.1% Trifluoroacetic acid and Acetonitrile as a gradient mobile phase. The flow rate was adjusted at 0.3ml/min with 1µl injection volume. The total analysis takes 7 minute with good resolution and minimal tailing.

Time	Flow	% A (0.1 % TFA)	% B (ACN)	Curve
-----	0.3	79	21	Initial
2.0	0.3	79	21	6
2.5	0.3	70	30	6
5.0	0.3	45	55	6
5.0	0.3	79	21	6
7.0	0.3	79	21	6

Table 1: Gradient programming for proposed method

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ANTIMALARIAL DRUG DISCOVERY: OPTIMIZATION OF BIOLOGICAL ACTIVITY AND PHYSICOCHEMICAL PROPERTIES OF PROTOZOAN GROWTH INHIBITORS USING TARGET CLASS REPURPOSING

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Neglected and tropical diseases affect a large proportion of the world's population and represent a significant unmet medical need, primarily due to low financial incentives for costly and risky drug discovery efforts. Streamlined drug discovery approaches are therefore needed, and, with this in mind, our laboratory implements a “Target Class Repurposing” approach aimed atreducing resource requirements for drug discovery. In which,essential parasite targets classeswith human homologs previously pursued for drug discovery are identified, and existing knowledgeof established chemical inhibitors for these human targets is reused. Applying this approach we recently reported discovery of highly active anti-malarial agentsderived from lapatinib, an approved tyrosine kinase inhibitor. Although highly potent, these compounds display poor physicochemical properties. Our ongoing efforts to optimize activity and physicochemical properties for this disease will be discussed, and promising new lead compounds for malaria will be presented.

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MULTICOMPONENT SYNTHESIS OF CHROMENOPYRIMIDINONE VIA BIGINELLI REACTION AND THEIR ANTI-INFLAMMATORY ACTIVITY

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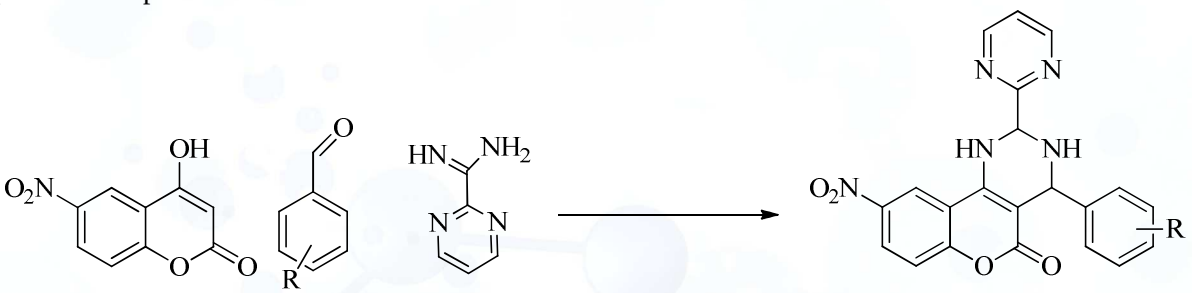
Multicomponent reactions are persuasive approach for developing a chemically diverse set of heterocyclic scaffolds with high yield. To this end, synthesis of a series of new 9-nitro-3,4-dihydro-1H-chromeno[4,3-d]pyrimidin-5(2H)-one has been accomplished by multicomponent cyclocondensation reaction of 6-nitro-4-hydroxycoumarin, various substituted aldehyde, and pyrimidine-2-carboximidamide using HCl as catalyst in methanol with up to 88% yield. The anti-inflammatory studies of the title compounds have also been evaluated. The detailed study will be presented in poster.



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THE SYNTHESIS OF SOME NOVEL PYRAZOLE DERIVATIVES

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All the three pyrazole derivatives have been synthesized through novel synthetic process. Firstly, 4-(p-tolylthio)-1H-pyrazol was synthesized by reacting 3-methyl-1-phenyl-1H-pyrazol-5-amine with N-chlorosuccinimide and 4-methylthiophenol. Similarly, 3-(5-amino-3-methyl-1-phenyl-1H-pyrazol-4-yl)isobenzofuran-1-(3H)-one was synthesized by condensing 3-methyl-1-phenyl-1H-pyrazol-5-amine and 2-formylbenzoic acid in water. Moreover, 4,5,6,7-tetrahydro-1H-pyrazolo[3,4-d]pyrimidine derivatives were also prepared via C- and N-alkylation reaction of 3-methyl-1-phenyl-1H-pyrazol-5-amine, corresponding primary amine and formaldehyde. All the synthesized compounds were well characterized by IR, ^{1}H NMR and ^{13}C NMR, Mass spectrometry. To know the absolute configuration of the synthesized compounds, X-Ray crystallography study was also performed by developing the crystal of the compounds.

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A COMPREHENSIVE STUDY ON FORCE DEGRADATION BEHAVIOR TO SIGNPOST THE STORAGE CONDITION OFA NEW ANTIMUSCARINIC DRUG AND CHROMATOGRAPHIC METHOD SWITCH FROM HPLC TO UPLC

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The objective of this study was to signpost the storage condition of FesoterodineFumarate by a comprehensive force degradation study. The second most potential objective to transfer chromatographic method from conventional HPLC to a new generation instrument UPLC was to develop a solvent free, fast and sensitive isocratic assay method. Chromatography was carried out on an Aquity UPLC HSS T3 @C18 column (50×2.1 mm, particle size 1.7 µm) and HPLC column Phenomenex Luna 5µ C18 with 250x4.6 mm, Particle size 5 µm. The major advantage of the Aquity UPLC HSS T3 column is that, 100% aqueous mobile phase can be used for elution. The mobile phase consisted of 0.1% OPA in water and methanol (95:5 v/v) and (90:10 v/v) at a flow rate of 0.30 mL/min and 1.0 mL/min at 30^0 C column temperature for UPLC and HPLC respectively. The detection was achieved at 220 nm for both instruments. The method validation performed according to the ICH guideline, where results of all validation parameters meet with acceptance criteria.

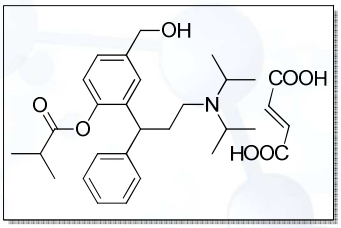

Fig: Structure of a new antimuscarinic drug Fesotrodinefumarate

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SYNTHESIS AND EVALUATION OF LIQUID CRYSTAL BEHAVIOR OF A NOVEL HOMOLOGOUS SERIES:4-(4-N-ALKOXY BENZOYLOXY) B-METHOXY ETHYL BENZOATES

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Abstract: A novel homologous series of liquid crystals, viz., 4-[4'-n-alkoxy Benzoyloxy β-Methoxy Ethyl Benzoates has been synthesized. The series consists of eleven homologs. The methyl to butyl derivatives are not liquid crystalline and the rest of the homologs are enantiotropic liquid crystals. The octyl and decyl derivatives of the series are enantiotropically smectogenic in addition to nematogenic in character, but the Pentyl, hexyl, dodecyl, tetradecyl, and hexadecyl homolog derivatives of the series are only nematogenic without the exhibition of a smectic phase. The transition temperatures of the novel substances were determined by optical polarizing microscopy equipped with a heating stage. A plot of transition temperatures versus the number of carbon atoms present in the n-alkoxy terminal chain represents the phase behavior of the series. An odd-even effect is observed for the nematic-isotropic transition curve. The textures of the nematic phase are of a threaded or Schlieren type and those of the smectic A phases are typical. Analytical and spectral data agree with the molecular structures. The smectic and nematic thermal stabilities are 179.0 ºC and 196.28 ºC, respectively. The smectic phase commences from the octyloxy homologue and Nematic mesophase commences Pentyl homologue. Smectogenic phase lengths vary from 15.0 ºC to 17.0 ºC and the nematogenic phase lengths vary from 7.0 ºC to 33.0 ºC. The series is predominantly nematogenic and partly smectogenic with considerable mesophase length and a middle-ordered melting type. The liquid crystal properties of the present series are compared with structurally similar homologous series.

Keywords: Liquid crystal; smectic; nematic; mesomorphic; thermotropic

P-96

AN IMPROVED ASSAY METHOD FOR THE ESTIMATION OF TICAGRELOR HYDROCHLORIDE BY REVERSE PHASE LIQUID CHROMATOGRAPHY

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Abstract: The current investigation was carried out to develop and validate a fairly simple, accurate, precise, reproducible and robust RP-HPLC method for the estimation of Ticagrelor Hydrochloride. The separation was achieved using Agilent Infinity 1220, Infinity Fast-LC (Pressure limit up to 600 bars) with auto sampler and PDA detector.Chromatographic analysis was performed on ZORBAX Eclipse Plus 300SB C18 (250 x 4.6mm, 5.0 micron, PN 880995-902) column. Mobile phase consist of (A) Acetonitrile: (B) 20mM Potassium dihydrogenortho phosphate buffer (40:60 v/v) at a flow rate of 1.0 ml/min. The method showed linear in the mentioned concentrations having line equation y = 22.848x + 1.3214 with correlation coefficient R2 of 0.9995. The recovery values for Ticagrelor ranged from 99.63% to 100.34%. The % RSD was 0.49% and 0.54%, respectively for intraday and interday precision. The limit of detection and limit of quantification were 0.05µg/mL and 0.20µg/mL respectively. Newly developed method was statistically validated for accuracy, precision, linearity and solution stability; hence it is directly applicable for the estimation of Ticagrelor up to trace level in routine analysis.

P-97

MICROWAVE ASSISTED GREEN APPROACH FOR THE SYNTHESIS OF FUSED HETEROCYCLES*VIA* GROEBKE-BLACKBURN-BIENAYMÉ MULTICOMPONENT REACTION AS POTENT ANTICANCER AGENTS

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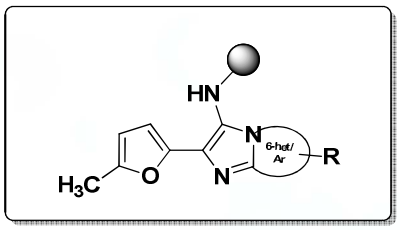

Cancer remains one of the most difficult diseases to treat and is one of the leading causes of human mortality.[1] Developing new anticancer drug and more effective treatment strategy to treat cancer is of great challenge for the medicinal chemist. Imidazole and its derivatives have attracted considerable interests in recent years for their versatile properties in chemistry, biology and pharmacology, especially antitumor activity.[2][3]Most interestingly, more recent literature survey has revealed that attachment of a furan moiety can significantly enhance the antitumor activity of candidate compounds.[4]A series of novel hybrid compounds between imidazole and furan has been synthesized by microwave assisted green approach following a Groebke-Blackburn-Bienaymé MCR[5] and evaluated *in vitro* against a panel of NCI-60 human tumor cell lines under developmental therapeutic program.

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P-98

A COMPARATIVE X-RAY CRYSTALLOGRAPHIC STUDY OF NOVEL MANNICH BASES OF 1,4-DIHYDROPYRIDINES

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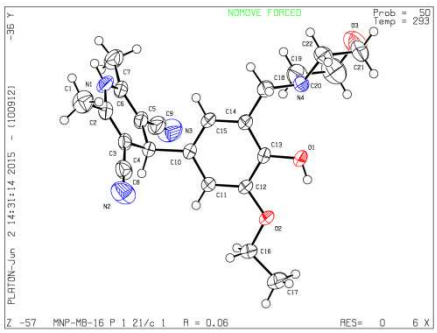
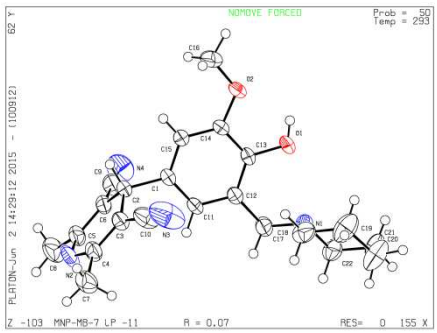
The novel mannich bases are synthesized by Mannich reaction of 1,4-dihydropyridines containing one hydroxyl group at C-4 position and one ethoxy group also introduced along with hydroxyl group on C-4 position of phenyl ring and various secondary amines. Compound $C_{22}H_{26}N_4O_3$ crystallizes in monoclinic crystal system with P21/c (#14) space group with cell parameters a = 16.816(2) Å, b = 10.285(8) Å, c = 12.633(9) Å and Z=4 while compound $C_{22}H_{26}N_4O_2$ crystallizes in primitive triclinic system with space group P-1(#2), cell parameters a = 6.098(7) Å, b = 10.526(2) Å, c = 17.264(2) Å and Z=2





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P-99

Development of a novel solvent selective and green synthetic protocol for post-Ugi intramolecular cyclization

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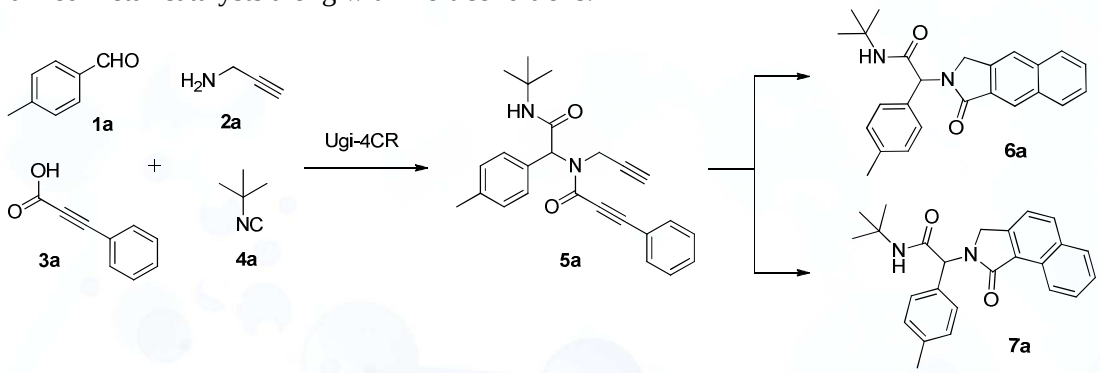
Multi-component reactions (MCR), like Ugi-4-CR, inherently bequeath molecular diversity and complexity in a single step; and subsequent post-Ugi cyclization provide a powerful way to synthesize novel heterocycles in an unprecedented and economic synthetic pathway.However the tuning of selective ring closure is an ever-standing challenge in synthetic organic chemistry; and requires use of specialized metal-catalysts along with inert conditions.



Herein we report a solvent tuneableand metal-free [4 + 2] cycloaddition approach via intramolecular Csp^2–H functionalization. Protic and aprotic solvents trigger different reaction pathway, delivering two exclusive and diverse heterocycles, *N*-subsitutedbenzo[e]-or [f]isoindolones in high yields. The protocol is highly atom economical with water being the only by-product. All the newly synthesized compounds are well characterized by sophisticated spectroscopic techniques.

P-100

SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL EVALUATION OF SOME NOVEL MANNICH BASES OF 1,4-DIHYDROPYRIDINE DERIVATIVES

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1,4-Dihydropyridine derivatives (1,4-DHPs) are versatile intermediates in organic synthesis. Moreover, compounds based on this heterocycles play key roles in therapeutic and bioorganic chemistry as calcium channel modulators. Many natural products as well as first, second, and third generation calcium channel blockers such as nifedipine, nitrendipine, felodipine, amlodipine and nisoldipine are 1,4-DHPs. Here we to present synthesis of a series of novel Mannich base of 1,4-dihydropyridin. All the compounds were synthesized using substituted hydroxyl benzaldehydes, 3 amino crotononitrile, formaldehyde and various secondary amines.

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P-101

A SIMPLE, RAPID AND SENSITIVE ASSAY METHOD FOR THE SIMULTANEOUS DETERMINATION OF THE FIVE POTENT ANTIDEPRESSANT DRUGS BY RP HPLC-UV

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The objective of the present work was to develop and validate an assay method for the simultaneous determination of the salt of five potent antidepressant drugs like; Nortriptyline, Bupropion, Milnacipran, Fluoxetine and Sertraline by a single isocratic method, was carried out with the help of High performance Liquid Chromatography (HPLC) using a UV detector using water: acetonitrile: glacial acetic acid (GAA): tri ethyl amine (TEA) in proportion of (58: 40: 1: 1). The satisfactory retention of all these five drugs was observed within 15min. of total runtime by a stationary phase of SunFire C18 (4.6 x 250 mm, 5µm) with 0.90ml/min of flow rate at 215nm of detection wavelength. The linearity of these drugs was obtained in the concentration range of 6 to 42µg/ml with Correlation coefficient ≥ 0.9998. The detection limit value of these drugs is 0.16µg/ml which shows the sensitivity of the method. The % relative standard deviation value of validation parameters was within a limit as per ICH guideline, which proves the method is fast, precise and reproducible.

P-102

THE QUANTITATIVE UPLC METHOD FOR DETERMINATION OF SIMVASTATIN (MARKETED FORMULATIONS) WITH FORCED DEGRADATION STUDY

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The present investigation describes the quantitative UPLC method for determination of simvastatin with forced degradation study. Simvastatin belongs to cholesterol lowering lactones category. It is also used for cardiovascular diseases along with cholesterol maintenance [1][2][3]. In the present method, the chromatographic analysis was performed using Acquity BEH C18 (2.1 mm id X 100mm, 1.7um particle size) column. The separation was achieved with isocratic mobile phase consisting Acetonitrile and 0.1% Orthophosphoric acid (pH 2.5) in the ratio of (75:25, %v/v). The flow rate has been set at 0.35ml/min with 2 µl injection volume. The detection was monitored at 238nm wavelength. The total analysis takes 5 minutes.

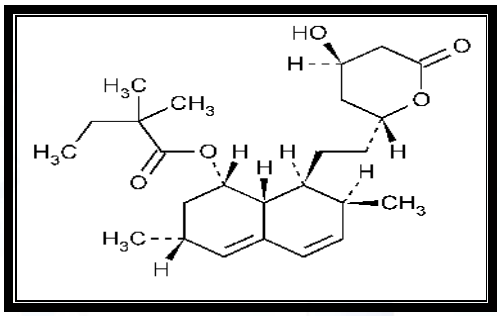

Figure 1: Structural formula of Simvastatin

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P-103

'IN SILICO' IDENTIFICATION OF MIRNA ENCODED BY *CHIKUNGUNYA* VIRUS AND TARGET PREDICTION IN HUMAN

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Abstract: *Chikungunya* virus, also referred to as CHIKV, is a member of the *alphavirus* genus, and *Togaviridae* family. It is a viral disease transmitted to humans through infected mosquitoes. The pathogenesis of *Chikungunya* infection in humans is still poorly understood, despite recent outbreaks. It was hypothesized that CHIKV might contain miRNA which mediates post transcriptional gene silencing of target human proteins. *'In Silico'* analysis of *Chikungunya* virus genome (Name of Software used: VMir Analyzer, VMir Viewer, Mfold, MATUREBAYES, VirMir Database, Mir.Tar.Human, Bio-GPS Profiles) was done to investigate the presence of miRNA and further interaction of *Chikungunya* viral miRNA with human target m-RNA. Though strict stringency and filtration parameters were applied, Software analysis gave out surprising results. Further, correlation studies of *Chikungunya* Symptoms and miRNA target protein was done that suggested the success and reliability of *'In Silico'* results. Additionally, virtual screening or molecular modeling will be performed to go ahead for therapeutic studies. The detail studies will be discussed in poster.

P-104

SIMULTANEOUS QUANTIFICATION OF TOLPERISONE AND PARACETAMOL BY HPTLC

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A simplest and rapid HPTLC method has been developed and validated for the simultaneous estimation of Tolperisone and Peracetamol in combined dosage forms. The method employs thin-layer chromatography (TLC) aluminum plates precoated with silica gel 60 $_{F254}$ as the stationary phase, while the solvent system was ethyl acetate: methanol: glacial acetic acid (5:5:0.3, %v/v/v). The R_f values were observed to be 0.65 ± 0.02 and 0.82 ± 0.02 respectively for Peracetamol and Tolperisone. The separated band was analyzed in absorbance mode at 272 nm wavelength with 2µl injection volume. The method was validated with respect to System suitability, Linearity, Accuracy, Precision, LOD and LOQ study.

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P-105

DIVERSITY ORIENTED EXPEDIENT ROUTE FOR THE SYNTHESIS OF 3-TETRAHYDROPYRIMIDINYL-COUMARINS VIA MCR

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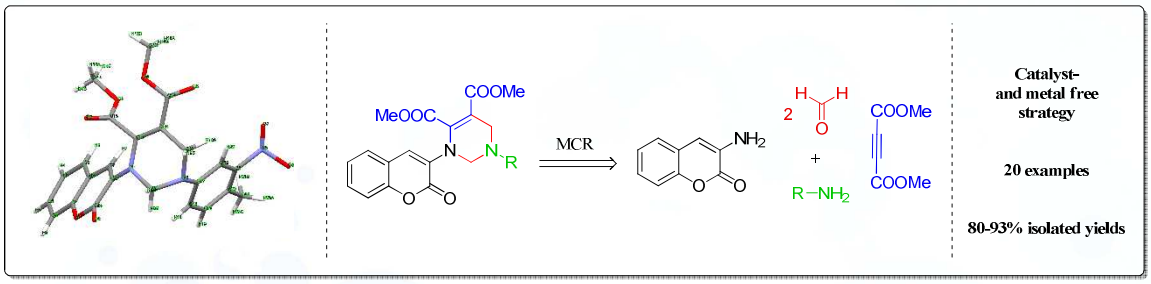
Abstract: A practical,mild and high yielding synthetic approach for the synthesis of unknown tetrahydropyrimidinyl substituted 3-coumarins as hybrid scaffolds, potentially useful NCE's is described via metal- and catalyst-free multicomponent cyclization. The enhanced nucleophilicity of 3-amino coumarins *versus* 4-amino coumarin is explained via the difference in ^{13}C NMR δ values (Δδ) of vinylic carbons. X-ray crystal analysis defines the structure of a representative set of example.



P-106

The synthesis and biological evaluation of new DNA-directed alkylating agents, phenyl N-mustard-4-anilinoquinoline conjugates containing a urea linker

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The synthesis of a series of phenyl N-mustard-4-anilinoquinoline conjugates was done to study their anti-tumorigenic effects.[1][2] These agents were prepared by the condensation of 4-[N,N-bis(2-chloroethyl)amino]phenyl isocyanate with 6-amino-4-methylamino or 4-anilinoquinolines.[3][4] The structure activity relationship (SAR) studies revealed that the C2-methylquinoline derivatives were generally more cytotoxic than the C2-phenylquinoline conjugates in inhibiting the cell growth of various human tumor cell lines in vitro. However, the methylamino or aniline substituents at C4 of quinoline did not influence the cytotoxic effects. The title conjugates were capable of inducing DNA cross-linking and promoting cell-cycle arrest at the G2/M phase. This study demonstrates that phenyl N-mustard-4-anilinoquinoline conjugates are generally more potent than phenyl N-mustard-4-anilinoquinazoline conjugates against the cell growth of various tumor cell-lines.

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P-107

SYNTHESIS AND ANTICANCER ACTIVITY OF UREA AND THIOUREA DERIVATIVES BEARING [1,2,4]TRIAZOLO[4,3-a]PYRIDINE SCAFFOLD

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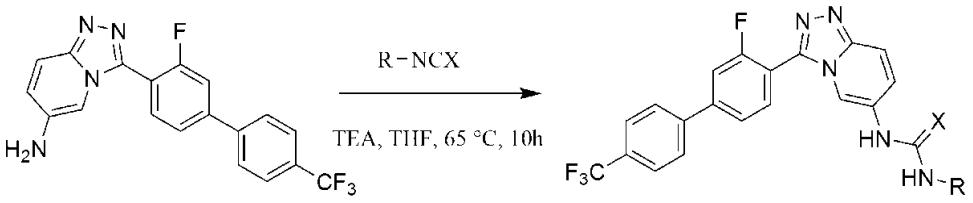
Abstract: Heterocyclic compounds are very widely distributed in nature and are important constituents found in the most commercial drugs. Among various heterocyles, [1,2,4]triazolo[4,3-a]pyridins are privilege scaffolds exhibiting a broad spectrum of bioactivity including antibacterial, anti-TB, antiviral etc. In our ongoing interest for developing novel anticancer based on pyridine nucleus, we have developed a library of new [1,2,4]triazolo[4,3-a]pyridins by incorporating Urea & thiourea derivatives to access their bioactivity. We found that several of these derivatives exhibit potential anticancer activity against Human breast carcinoma (MDMB-231) & Prostate Cancer Cell (PC-3) growths. Compound KM-115 and KM-121 showed GI50 in micro molar range warrant it's further development as anticancer drug.



P-108

Synthesis and Characterization m-tolylpyrimidin-2-ol and m-tolyl pyrimidine-2-thiol Derivatives

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Some new substituted m-tolylpyrimidin-2-ol and m-tolylpyrimidine-2-thiol derivatives have been synthesised from 4-Methyl acetophenone react with different aldehyde and prepare chalcone intermediate in presence of NaOH in Methanol solvent and this intermediate react with urea and thiourea to isolate different m-totyl pyrimidine-2ol and m-tolylpyrimidine-2-thiol derivatives their chemical structures have been confirmed by IR, 1H NMR, and MASS and by elemental analysis. Investigation of antimicrobial activity of compound was done by the disk diffusion technique. The synthesized selected compounds were evaluated for their anti-inflammatory and analgesic activity.

Keywords: Pyrimidine, Chalcones, Anti-inflammatory activity, Analgesic activity.

P-109

Design, synthesis and anti-tubercular activity of novel *N*'-benzylidene-2-(quinolin-6-yloxy)propanehydrazide analogs

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Abstract: Fifteen novel *N*'-benzylidene-2-(quinolin-6-yloxy) propanehydrazide analogs were designed as potential anti-tubercular agents using molecular hybridization approach [1, 2] and evaluated *in-silico* for drug likeness behaviour [3]. Designed compounds were synthesized, purified, characterized and *in-vitro* evaluated for anti-tubercular activity (against *M. tuberculosis* H37Ra) [4, 5]. Four compounds (**6h**, **6j**, **6l** and **6m)** exhibited significant anti-tubercular activity with MIC values below 20 µg/mL in which two most active compounds **6j** and **6m** exhibited MIC values 7.70 and 7.13 µg/mL respectively. Structure Activity Relationship (SAR) study of the tested compounds revealed that, electron withdrawing group of moderate to large size especially at *para* position of phenyl ring significantly increased the potency against *M. tuberculosis*. All compounds were also evaluated for cytotoxicity against human lung fibroblast cells [6]. But, none of the compound exhibited cytotoxicity at tested concentration (512 µM). Over all study can be helpful for further lead optimization as well as designing of new anti-tubercular agents.

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P-110

Effects of surfactants on the oxidation of Methyl Red

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Abstract: The kinetics of oxidation of aromatic azo dyes viz., methyl red (MR) by V (V) has been investigated in aqueous sulphuric acid media. The reaction studied spectrophotometrically in aqueous sulphuric acid medium is first order in vanadium (V) and methyl red (MR). Plots of k_{obs} versus $[H^+]$ are linear with positive intercepts on k_{obs} axes, suggesting the formation of a complex between vanadium (V) and dye. The oxidation of methyl red (MR) by V (V) in aqueous sulphuric acid media in the presence of non-ionic surfactants at different temperatures has been investigated. The activation and thermodynamic parameters have been calculated.

P-111

Nanoscaled iron-zirconium mixed oxide for the adsorptive-removal of Cr(VI) from industrial wastewater: *An Ecofriendly approach*

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Iron-zirconium mixed oxide nanoparticles have been studied for their adsorption efficiency towards Cr(VI). Nanoscaled iron-zirconium mixed oxide were synthesized using precipitation techniques and characterized by elemental analysis, TG/DT analysis, FTIR, UV-Visible spectroscopy, XRD pattern and SEM techniques.The synthesized material was found to be effective adsorbent for the adsorption of Cr(VI). The Cr(VI) was taken as $K_2Cr_2O_7$.A fixed amount of synthesized adsorbent was added to a definite volume of $K_2Cr_2O_7$ solutions under optimized conditions such as adsorption time, concentration of $K_2Cr_2O_7$, amount of adsorbent, temperature and pH. The mixture was allowed to attain equilibrium.Small aliquot was withdrawn from this equilibrium mixtureat different timeintervals. The concentration of $K_2Cr_2O_7$ in supernatant has been determined using UV–Vis spectrophotometery.

The synthesized nanoscaled iron-zirconium mixed oxide showed a high efficiency for the adsorption of Cr(VI). The adsorption of Cr(VI) was found to be highly dependent on pH. The synthesized nanomaterial showed nearly 85% adsorption of Cr(VI). The adsorption data was found to follow Langmuir adsorption isotherm.

P-112

An Efficient Dehydrogenative Fujiwara-MoritaniAlkenylation

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Carbon-Carbon or Carbon-heteroatom bond forming reaction under C-H functionalization strategy has become a frontier in current synthetic chemistry. In modern era, alkenylation reaction using transition metal catalyst has a great synthetic application in various field viz. pharmaceuticals, natural products, agrochemicals etc. Alkenylation reaction using organometallic compounds require prefunctionalisation of substrate and the reaction is air and moisture sensitive too. Fujiwara-Moritani Reaction, Alkenes are generated by intermolecular dehydrogenative reactions between aromatic and olefinic compounds but herein we are reporting Fujiwara-Moritani reaction without any external acids and pressurized gas.

Keywords: Transition metal catalyst, C-H functionalization, Fujiwara-Moritani reaction

P-113

SIMULTANEOUS QUANTIFICATION AND STABILITY STUDY OF TOLPERISONE HCL AND PARACETAMOL USING UPLC

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Abstract: In the present work, Tolperisone HCl and Paracetamol were quantified by ultra-fast and sensitive isocratic RP-UPLC method. Developed method was validated as per ICH guidelines. Chromatographic separation was done isocratically on Acquity UPLC BEH C_{18} (50 mm ×2.1 mm, particle size 1.7 µm) and detection utilizing PDA detector at 254 nm with injection volume of 2.0 µL. Mobile phase used for chromatographic separation was 0.1% Ortho-phosphoric acid in water and acetonitrile (70: 30 v/v) as at a flow rate of 0.20 mL/min and 35 ºC column temperature. Simultaneous analysis was done in 4 min with elusion of Tolperisone HCl and Paracetamol at 1.396 and 2.625 min respectively. Along with faster and simultaneous analysis, linear calibration curve was found over the wide concentration range of 6.0 µg/mL to 54.0 µg/mL and 20.0 µg/mL to 180.0 µg/mL for Tolperisone HCl and Paracetamol, respectively. This simple and less time consuming method was cost effective and have better quality control over the existing methods.

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Enzymatic separation of epimeric 4-*C*-hydroxymethylated furanosugar: synthesis of bicyclic nucleosides

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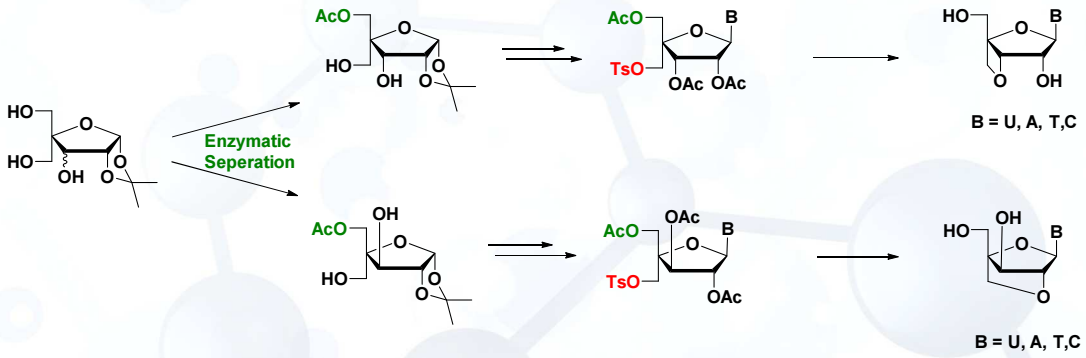
The synthesis of clinically useful modified nucleosides is an arduous task and requires selective manipulation of almost identical multiple functionalities. The use of biocatalysts has become an attractive alternative for conventional chemical methods due to their selectivity and high efficiency.

Our continued interest in study of lipase catalyzed regio- and stereo-selective reactions on different bioactive compounds led us to develop an efficient and high yielding protocol for the separation of 4-*C*-hydroxymethyl-1,2-*O*-isopropylidene-*α*-D-*xylo*/*ribo*furanose derivatives through regioselective acetylation catalyzed by lipases. The lipase, Novozyme®-435 catalyzed selective acetylation led to the transfer of acetyl group at C-5 position in both the derivatives. The 5-*O*-acetate of 4-*C*-hydroxymethyl-1,2-*O*-isopropylidene-*α*-D-*xylo*furanose and 4-*C*-hydroxymethyl-1,2-*O*-isopropylidene-*α*-D-*ribo*furanose are of different polarity and thus can be easily separated by column chromatography. The structure of monoacetylated 5-*O*-acetyl-4-*C*-hydroxymethyl-1,2-*O*-isopropylidene-*α*-D-*xylo*furanose and 5-*O*-acetyl-4-*C*-hydroxymethyl-1,2-*O*-isopropylidene-*α*-D-*ribo*furanose were confirmed by X-ray crystallographic data analysis. Separated intermediates were further used for convergent synthesis of series of bicyclic nucleosides.



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P-115

Chemo-enzymatic Access to Therapeutically Modified Sugar Nucleosides

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Nucleosides are among the most widely studied fundamental building blocks of biological system that are used as therapeutic agents to treat cancer, fungal, bacterial and viral infections. The conformational behaviour of natural or modified nucleosides has demonstrated great importance in terms of their metabolic pathways and interactions with the biological targets. This has resulted in the synthesis of chemically modified nucleoside analogues having conformationally restricted pentofuranose ring. Prominent among these are the Spironucleosides and Locked nucleic acid (LNA).

Since, the synthesis of clinically useful modified nucleosides is an arduous task and requires selective manipulation of multiple functionalities present in sugars or nucleosides, the use of biocatalysts in the synthesis of nucleoside analogues has become an attractive alternative for conventional chemical methods due to their selectivity and high efficiency. We herein report the chemo-enzymatic synthesis of novel 3′-azido-spiro and bicyclonucleosides. The full details of synthetic scheme will be presented during the poster session.

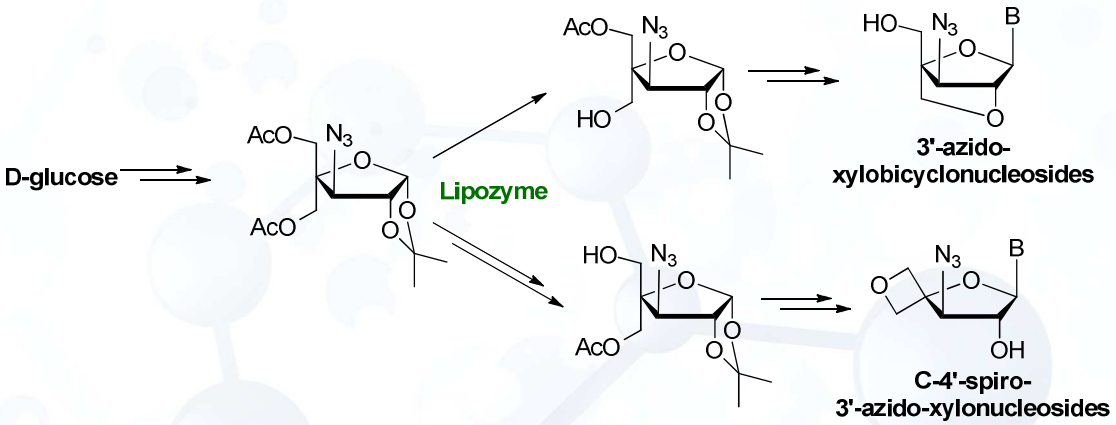

Figure 1. Chemo-enzymatic synthesis of novel 3′-azido-spiro and bicyclonucleosides.

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P-116

Chemo-enzymatic access to *α*-L-LNA monomers

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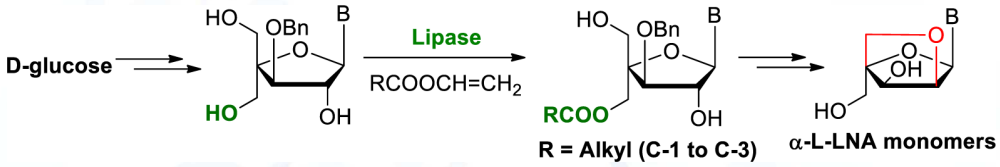
Over the past 35 years, different types of modified nucleosides and oligonucleotides have been synthesized for their use in drug discovery. Among numerous known modifications, enhancement of conformational rigidity of sugar moiety in nucleosides by the introduction of a 2′-*O*,4′-*C* methylene-linkage, such as in locked nucleic acids (LNA), has been found to be very useful for antisense applications. α-L-LNA (Scheme 1) is a promising DNA-like modification which is obtained by inverting all the sugar substituents of LNA except the nucleobase. This modification has slightly lower binding affinity than LNA, but exhibited excellent stability against nucleases as well as RNase H recruitment. α-L-LNA gapmer have demonstrated superior efficacy over the parent LNA or LNA analogue gapmers towards *in vitro* and *in vivo* gene knockdown without producing hepatotoxicity.

In the present work, Lipase catalyzed regioselective acylation of one of the three hydroxyl functions in the case of 3-*O*-benzyl-4-*C*-hydroxymethylated xylonucleosides has been achieved and utilized for efficient synthesis of *α*-L-LNA monomers (Scheme 1). The detailed synthetic scheme will be presented during the poster session.



Scheme 1. Chemo-enzymatic synthesis of *α*-L-LNA monomers; B = nucleobase.

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P-117

LARVICIDAL ACTIVITY OF ESSENTIAL-OIL-LOADED NANOEMULSIONS AGAINST FILARIASIS VECTOR

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Abstract: Mosquitoes play predominant role as vectors of pathogens causing dreadful diseases like malaria, dengue fever, yellow fever, filariasis, chikungunya and japanese encephalitis [1]. *Culex quinquefasciatus* is one of the important vectors of filarial parasite *Wuchereria bancrofti* [2]. Potential risks associated with the use of toxic synthetic pesticides lead to an abrupt and urgent necessity to develop ecofriendly and more efficient alternative to replace these synthetic pesticides [3]. Essential oils are bio-based pesticides with significant larvicidal properties [4]. Nanoemulsions are dispersions of oil and water with droplet size in the range of 10–100 nm [5]. Plant essential oil based nanoemulsion was formulated by ultrasound cavitation method. Droplet size of optimized nanoemulsion was 24 nm. Formulated nanoemulsion demonstrated dose and time dependent larvicidal activity against *Culex quinquefasciatus*. Complete loss of larval viability was observed within in 6 hr of interaction with 100 ppm nanoemulsion, whereas it took 18 hr and 24 hr when interacted with 75 ppm and 50 ppm of nanoemulsion respectively. Formulated nanoemulsion was observed to be an efficient larvicide against *Culex quinquefasciatus* even at very low concentration of 5 ppm. After 24 hr of interaction with 5 ppm of nanoemulsion, 50 % larva mortality was observed. Histological staining confirmed the damage caused by nanoemulsion treatment. Larvicidal activity of the plant essential oil nanoemulsion can be attributed to the lower droplet size of nanoemulsion and the bioactive component in the essential oil. Further, this nanoemulsion formulation can be used for mosquito vector control.

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P-118

Computational studies of benzimidazol-2-thiol as STAT3 inhibitors

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Abstract: Signal transducer and activator of transcription (STAT) proteins are a family of transcription factors that mediate gene expression in response to cytokines and growth factors.STAT3 regulates a variety of genes involved in cell proliferation, differentiation, apoptosis, angiogenesis, metastasis, inflammation, and immunity. The central role of aberrant STAT3 signaling in tumorigenesis has rendered STAT3, and, to a lesser extent, STAT5, as an attractive target in anticancer therapy. The purpose of this study was to apply molecular docking techniques to identify STAT3 inhibitors potential of benzimidazol-2-thiol derivatives. Autodock Vina was used for docking studies against 1BG1 protein. S31-201 is a selective chemical probe inhibitor of STAT3 which was used for comparision of binding energy score. The binding energy showed by the derivatives is comparable to the standard used. Molecular docking analysis suggested that compounds might putatively function as an inhibitor of STAT3 dimerization by binding to the SH2 domain.

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Synthesis of novel 2, 5-di substituted 1, 3, 4-oxadiazole analogs as a potent antibacterial and antitubercular agent

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Abstract: A series of 2, 5-di substituted-1, 3, 4-oxadiazole scaffold were designed, synthesized and evaluated antibacterial and antitubercular activity. Different (4a-k & 5a-k) 1, 3, 4-oxadiazole derivatives synthesized using substituted hydrazide and carbon disulphide in a basic media. The reactions were performed under conventional heating with higher yields. All the synthesized compounds were characterized by their spectral study (IR, MS, ^{1}H and ^{13}C NMR) and were tested for their antibacterial and antitubercular activities. The compounds 4b, 4i and 5h exhibited significant activity against *S. aureu*, 4e and 5i against *P. aeruginosa*, 4e, 4h and 5f against *E. coli*, 4g, 4h and 5j against *C. albicans* and 4g, 4i and 5j against *A. niger*. The compounds 4a, 4i, 5b and 5i exhibited significant activity against $H_{37}Rv$ *strain of M. tuberculosis*. Rest of the synthesized compounds showed moderate to poor activity against tested species with compared to standard.

P-120

Synthesis of novel (4-bromophenyl)(3-(4-ethyl-2,5-dimethoxyphenyl)-5-phenyl-1*H*-pyrazol-1-yl)methanone analogs as a potent antibacterial and antitubercular agent

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Abstract: In present development of drug research, pyrazole and its derivatives are being considered as useful and promising leads due to their potentials to exhibit biological activities such as antibacterial and antitubercular activities. Different pyrazole derivatives (4a-m) were synthesized by cyclization of substituted chalcones with hydrazide. The reactions were performed under conventional heating. All the reactions were accelerated in basic conditions under conventional heating, with higher yields. All the synthesized compounds were characterized by their spectral study (IR, MS, ^{1}H and ^{13}C NMR) and were tested for their antibacterial antitubercular activities. The compounds 4b, 4i and 4l exhibited significant activity against *S. aureu*, 4e and 4h against *P. aeruginosa*, 4e and 4h against *E. coli*, 4g, 4h and 4j against *C. albicans* and 4g, 4i and 3j against *A. niger*. The compounds 4a, 4i and 4k exhibited significant activity against *H_{37}Rv strain of M. tuberculosis*. Rest of the synthesized compounds showed moderate to poor activity against tested species with compared to standard.

P-121

Sonochemical synthesis of nanoparticles of the coordination complex and act as biologically active agent

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Abstract: Nano-sized Co(III) coordination complexes, $[Co(NH_3)_5N_3]Cr_2O_7$ (1) and $[Co(NH_3)_5N_3]CrO_4$ (2) has been synthesized by sonochemical method. These nano sized complexes were initially characterized by elemental analyses followed by spectroscopic analyses like IR and UV/Visible spectroscopy. Morphology of nano-sized complexes was determined by SEM and their particle size was found with the help of Zeta-sizer.X-ray powder diffraction study was also used to identify the phase difference between nano structures and bulk complexes. These complexes evaluated against different microbial strains.

Keywords: Cobalt(III), Nano-structure of cobalt(III) complexes, Sonochemical synthesis, X-ray powder diffraction

P-122

Synthesis, characterization and antimicrobial screening of tetrahydropyrimidine derivatives

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Abstract: A series of tetrahydropyrimidine derivativeswere synthesized by the modified Biginelli and Hantzsch reaction. A mixture of *N*-(*2,4-dimethylphenyl*)-3-oxobutanamide, different substituted aldehyde and thiourea in methanol were refluxed to get the product of 4-(aryl)-*N*-(2,4-dimethylphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxamide**.** The structures of synthesized compounds were characterized by IR, ^{1}H-NMR, ^{13}C-NMR and mass spectrometry. The synthesized compounds were screened for their antimicrobial activity against different strains of Gram-negative (*E. coli* and *P. aeruginosa*) and Gram-positive (*S. aureus* and *S. pyogenus*) bacteria and selected fungi*C.albicans, A. niger and A. clavatus* using serial broth dilution method (Muller-Hinton broth dilution method).This synthetic pathway was modified reaction scheme and decreases the reaction time.

Keywords: Tetrahydropyrimidines, Biginelli reaction andHantzsch reaction, antimicrobial activity, MIC

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Herbal therapy for treatment of Dengue

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Abstract: This review emphasise a therapeutic effect of Carica papaya in treatment of dengue fever caused by *Aedes aegypti* mosquitohaving DENV-1, DENV-2, DENV -3, DENV-4 belongs to *flaviviridae family*and today affects a vast number of people in more than 100 countries andresponsible for more than 50% of deaths. In the absence of an effective antiviral drug to treat the disease, various treatments are being investigated but none is effective.Studies have indicated that the juice of the leaves of the C.papayaplant from the family *Caricaceae*is used in folk medicines and provide beneficial effect as anti-inflammatory agent that help to increase the platelet levels in these patients.Survey indicates that papaya leaf juice contain the enzyme chymopapin and papain that boost platelets(thrombocytes).Oral administration of the young leaf said to have a positive impact on thrombocyte count. Thusthis study concluded that C.Papaya leaf extract(CPLE) significantly increase the platelet count in patients. Further studies raise the possibility that this treatment is an important option in the future and large-scale studies establish usefulness of this natural product to treat dengue.

Keywords: Dengue, *Aedes aegypti*, papaya leaf, Oral Administration, Thrombocytecount.

P-124

Ophthalmic drug delivery using timolol loaded nanoparticles laden contact lenses using 3D Digital Inkjet Printing Technology

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Abstract: Glaucoma is commonly treated using eye drops, which is highlyinefficient due to rapid clearance (low residence time) from ocularsurfaceCiolino et al. [1].The objective of the research work was to provide sustained ocular delivery of timolol via 3-D digital inkjet printed contact lenses, to increase the ocular residence time of drug and to improve ocular bioavailability, withoutcompromising critical lens properties.The present work was to encapsulate timolol in ethylcellulose nanoparticles using double emulsion technology, and to disperse in HEMA monomer ink, which is commonly used as contact lens material. The formulation laden inks were printed on the surface of dry hydrogel contact lenses, using US patented 3-D Digital inkjet printing technology. To determine their suitability for extended wear, the printed contact lenses were characterized for physical and biological integrityPeng et al. [2]. The entrapped nanoparticles did not significantly alter the physical and surface characteristics of contact lenses. The *in-vitro* drug release study revealed that soaking batches and direct timolol loaded printed contact lenses showed therapeutic release up to 12 hours, with high drug loading of 100-117 µg. While microparticles laden printed contact lenses showed therapeutic release up to 24 hours with low drug loading of 20 µg. The printed contact lenses appeared safe in animal study. *In-vivo* study showed 66 hours sustained therapeutic effect (reduction in IOP), which suggest the potential of printed contact lenses.The study successfully demonstrates the potential of digital inkjet printing technology to print and deliver timolol for sustained delivery using contact lenses for the treatment of glaucoma.

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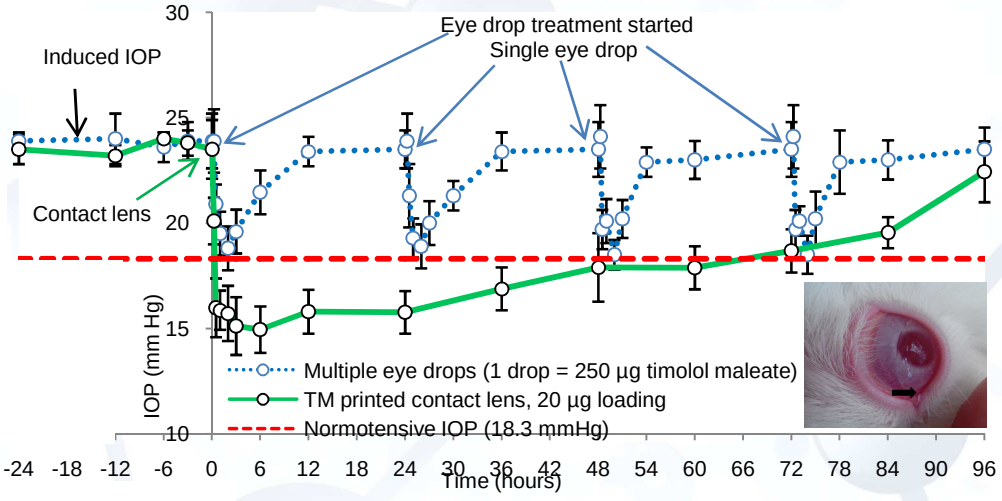

P-125

Evaluation of Phytochemical and Antioxidant activity of *Costus pictus* extracts

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Costus pictus D. Don, commonly known as 'Iinsulin Plant' is a member of Zingiberaceae family and is used as a munching dietary supplement for the treatment of various ailments in Southern India. Objectives of the present study were to evaluate the qualitative and quantitative phytochemical constitutions, antioxidant activity and HPTLC analysis of aqueous and methanolic extracts of dried leaves. The total phenolics and flavonoid contents were estimated by using the Folin-Ciocalteau and spectrophotometric methods respectively. Antioxidant activities of extracts were estimated by DPPH radical scavenging assay. The presence of various secondary metabolites such as alkaloids, phenols, flavonoids, steroids, tannins, saponins, amino acids and glycoside sugars were observed. Both the extracts showed higher total phenolic and flavonoid contents in compared to their standard controls (Gallic acid and Quercetin). The methanolic extract showed a significant *in vitro* antioxidant activity (>90% inhibition) as compared to aqueous extract and control (ascorbic acid). HPTLC and phytochemical activity results indicate the presence of a number of constituents. Due to the presence of antioxidant activity and various secondary metabolites, *Costus pictus* leaves would be an important candidate in pharmaceutical formulations and play a pivotal role in improving the human health by participating in the antioxidant defense system against free radical generation.

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POSSIBLE ANTI-ANGIOGENIC PROPERTY OF *BOMBAX CEIBA*

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Abstract: *Bombax ceiba* L. has been traditionally used in Ayurvedic medicine to treat various health problems. In the present study, *in vitro* shell less cultures of chicken (*Gallus gallus*) embryo (72 hours old) were treated with 0µg/mg 10µg/mg, 50µg/mg, 100µg/mg, 150µg/mg and 200µg/mg of aqueous as well as methanolic extracts from thorns of *Bombax ceiba L*. It was observed that number of capillary sprouts remained same at 0 hour, 3 hours and 6 hours post exposure at all concentrations studied. However there was significant increase in capillary sprouts in non treated embryos after 3 hours and 6 hours of growth. This implicates the ability of *Bombax ceiba* L. aqueous as well as methanolic thorn extract to inhibit angiogenesis and its promise in being developed as anti-cancer agent as well as its ability to stop, halt or reverse the onset of certain cancers.

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P-127

In-silico analysis of bacterial functional amyloids

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Amyloid proteins have been associated since long time with neurodegenerative diseases like Alzheimer's, Huntington's and many other Prion diseases [1]. Many unrelated proteins can assemble into amyloid folds indicating its evolutionary selection for different functions [2]. Unlike these, bacteria have also been identified recently for production and assembly of amyloids by directed pathways with functional physiological traits, termed as 'functional amyloids' that benefit the producing organism [3]. Such functional amyloids have been identified on many bacteria. Among these, 'curli' proteins on *E. coli* have been well studied [4]. Studies on Functional bacterial amyloids is an emerging field of study and are seen to perform various roles of strengthening cell surface interactions like adhesion, aggregation and biofilm formation [2,5,6] and for protection against host defences, thus playing potential role in animal and human infection [7,8]. In this study, we have analysed the structural variation and phylogenetic relation of various amyloid proteins by using their sequences available in the NCBI. Like many proteins, the bacterial functional amyloids also show a marked clustering in phylogeny, while the structural variance is significance. Amyloids from sporulating bacteria exhibited marked difference than the well studied amyloids from other pathogenic bacteria.

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Cubosomes: A Peerless Nanodrug Carrier

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Cubosomes are "Biological Capsules" that transport drug in safe and fast manner. Cubosomes are discrete, sub-micron nanostructured particles of biocontinuous cubic liquid crystalline phase[2]. Cubosomes are thermodynamically stable and have a structure like "honeycomb" with biocontinuous domain of water and lipid in which surfactant commonly used monoolein assembles into bilayer and twisted into 3D tightly packed structure[4]. This unique monostructure is biologically compatible and capable of controlled release of drug[5]. Overall cubosomes have great potential in drug nano formulations owing to their potential advantages including high internal surface area, cubic crystalline structure, relatively simple preparation method, biodegradability of lipids, ability to encapsulate hydrophobic, hydrophilic and amphiphilic substances, targeting and controlled release of bioactive agent. Cubosome formulated drugs have various routes of delivery[3]. Cubosomes generally have different internal cubic structure along with variant composition related to the drug holding modalities. Cubosome nanoparticles are a unique and intriguing self assembled material with enormous potential in areas as diverse as medicine, material science and consumer products.They have huge potential in drug nano formulations for melanoma therapy[1]. So while leaving normal tissues in the body virtually untouched, these therapies can be envisioned to specifically kill all cancer cells within the tumor. Nowadays, cubosomes are used as a drug carrier for 5- fluorouracil, fluconazole and odorranalectin.

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P-129

Identification and Characterization of Levansucrase Enzyme from Lactic Acid Bacteria

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Abstract: Lactic acid bacteria are Gram-positive, food-grade micro-organisms consisting of many genera, such as Lactococcus, Streptococcus, and Lactobacillus [1]. Lactic acid bacterial polysaccharides are of special interest because they may contribute to human health as prebiotics, or because of their antitumor, antiulcer, immune modulating, or cholesterol-lowering activity [2]. Levansucrase are involved in synthesis of fructan polymer known as levans [3]. The objective of this study is to identify and characterize the levansucrase enzymes from lactic acid bacteria obtained from dietary samples. On the basis of Biochemical tests and sucrose plate assay, a total of four strains AB, 0-1, 0-2 and 3-1 were showed both the tests positive. Further Dinitrosalicylic acid assay, thin layer chromatography and Native PAGE were performed to find thelevans producing ability. The entire assay indicated that only 0-1 strain hasability of producing polysaccharides. The 0-1 strain may harbour levansucrase enzymes.

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P-130

"Turn on" sensors for the intracellular detection of bioactive anions in the Hela cell line using Vitamin B_6 based receptor

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Abstract: Receptor **L** was developed that comprised of thiosemicarbazide with a vitamin B_6 group acting as chromogenic/fluorescence unit for the selective sensing of bioactive anions. The anion recognition ability of receptor **L** towards various anions was investigated by both spectroscopic (absorbance, fluorescence and ^{1}H NMR) and density functional theory calculation. The sensor showed stricking colour change from colourless to light yellow. The detection limit of **L** as a fluorescent 'turn-on' sensor for the analysis of F^- and AcO^- was estimated to be 0.10 µM. Receptor **L** it showed C=N isomerism . And it showed potential sensing of intracellular F^- ion in live HeLa cells.

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Graphite supported $BiCl_3$ as an efficient, heterogeneous and recyclable catalyst for synthesis of β-enaminones

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Abstract: Graphite supported bismuth trichloride is utilized as a green, efficient, heterogeneous and recyclable catalyst for the preparation of β-enaminones from amines in the presence of tetrahydrofuran at 66 ˚C temperature. Using this method, the title compounds are produced in high to excellent yields and in short reaction times. The catalyst was easily recovered from reaction system and readily reused with minimal loss of activity.

Keywords: β-dicarbonyl compounds, amines, enaminones, bismuth trichloride, graphite, tetrahydrofuran

P-132

Synthesis, characterization and dyeing performance of 2-amino 4-phenyl thiazole based bisazo disperse dyes

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Abstract: 2-amino-4-(4'-chlorophenyl)1, 3-thiazole was coupled with diazotized different primary amine which yielded mono azo dye. This monoazo dye was further diazotized and coupled with various substituted 2-hydroxy-N-(substituted)-benzamide to give corresponding bisazo dyes (D_1-D_8). The synthesized dyes were characterized by elemental analysis, UV, IR and ^{1}H NMR spectra. These bis azo dyes were applied on polyester fabric and their dyeing performance as well as fastness properties were evaluated.

Keyword: 2-amino 4-(4'-chlorophenyl) 1, 3-thiazole, substituted primary aniline, nitrosyl sulfuric acid, 2-hydroxy-N-(substituted)-benzamide, dyeing performance

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Characterization of *Bas3783* gene of *Bacillus anthracis* sterne

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Abstract: *Bacillus anthracis* is the etiological agent of anthrax. The major toxins involved in anthrax disease are PA, LF and EF. Production, delivery and action of these toxins in eukaryotic cells has been discovered. But, the mechanism of secretion of toxins from bacterial cells is not known. This secretion might be facilitated by some of the secretion system. Previously, homologous gene which code for subunits of Type IV Secretion System (TFSS) was reported in pX01 plasmid of *B.anthracis* [1], Recently, Grynberg et al. [2], also predicted gene homologues in *B. anthracis* which encodes TFSS component in other bacteria. Putative TFSS components are predicted to be present on the plasmids except one on chromosome [2]. Despite these bioinformatics leads, any genetic and/or molecular work has not been carried out to establish existence of TFSS in *B. anthracis* till date and also no one have tried to reveal the translocation mechanism of toxins PA, LF and or EF from cytoplasm to outside the cell. Vesicular secretion of toxin has been observed by Rivera et al.[3], but in non capsulated strain of *B. anthracis* whereas virulent strains are capsulated. Secretion of toxins in virulent encapsulated strain seems not likely the same. Out of several genes which are predicted to encode subunits of TFSS, we characterized *Bas3783*. This gene is located on chromosome and having homology with VirD4. We cloned, over expressed and also purified the recombinant protein. Polyclonal antibody was raised and interaction of recombinant protein with DNA was also observed.

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P-134

A One Pot, Solvent Free and Catalyst Free Synthesis of Substituted 2-Amino-5-Aryl-1,3,4-Oxadiazoles under Microwave Irradiation and their *In-vitro* Anti-malarial Study

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Abstract: A convenient one-pot, multi-component and solvent-free procedure for the preparation of substituted 2-amino-5-aryl-1,3,4-oxadiazoles (K4-K17) has been achieved. The method is a significant improvement over previously reported synthesis in the literature. Reaction of acid chlorides with hydrazine hydrate and isothiocynates under microwave-irradiation (MWI) afforded the corresponding 1,3,4-oxadiazole derivatives in high yields. With this protocol intramolecular cyclodesulfurization was occurring, due to the in-situ generation of HCl as a catalyst from the reaction, which afford substituted 2-amino-5-aryl-1,3,4-oxadiazoles exclusively. In general, the products precipitated from the reaction mixture, and were collected by filtration in almost pure form and there was no need to further purification. All synthesized compounds were characterized by FT-IR, proton and carbon NMR, mass spectroscopy and elemental analysis. Synthesised compounds were screened for *in-vitro* anti-malarial activity for *plasmodium falciparum*. From all synthesised compounds K5, K7, K12 and K14 showed more potent activity against *plasmodium falciparum* when compared with Quinine and Chloroquine as standard drugs.

P-135

Antimicrobial evolutionof novel coumarin hybrid thiosemicarbazone derivatives and their one pot synthesis

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Abstract: A convenient, one-pot, multi-component protocol for the preparation of 2-(1-(2-oxo-2*H*-chromen-3-yl)ethylidene)hydrazinecarbothioamide derivatives has been achieved. Here, firstly we have reported synthesis of 3-acetyl-2*H*-chromen-2-one using starch sulfuric acid and cellulose sulfuric acid as a biodegradable catalyst. Subsequently, we also carried out the reaction of isothiocynates, hydrazine hydrate and 3-acetyl-2*H*-chromen-2-one in the presence of catalytic amount of glacial acetic acid in refluxing ethanol to afford corresponding 2-(1-(2-oxo-2*H*-chromen-3-yl)ethylidene)hydrazinecarbothioamide derivatives in high to excellent yields. All synthesized compounds were characterized by FT-IR, ^{1}H-NMR, mass spectroscopy and elemental analysis. In addition, all synthesized compounds were screened for antimicrobial activity. All compounds were found to be good to excellent active against all four bacterial strain and one fungal strain.

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Needle Free Injection: A Novel Technology for Drug Delivery

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Needle-free injection devices have been available for humans since the about 80 years. Needle-free injection systems are novel ways to introduce various medicines into patients without piercing the skin with a conventional needle. They can take the form of power sprays, edible products, inhalers, and skin patches. Needle-free systems are designed to solve these problems making them safer, less expensive, and more convenient. In this delivery system an ultra-fine stream of medicinal product with pressure in a fraction of a second to the skin, subcutaneous tissue, and underlying shallow muscle without the use of a needle is done. Needle-free technology offers the benefit of reducing patient concern about the use of needle. Needle free injection gives very effective injections for a wide range of drugs to syringe and needle, results in less pain, and is strongly preferred by patients. Today, researchers are steadily developing technology that promises to make the administration of medicine more efficient and less painful.

Keywords: Needle Free Injections, Novel drug delivery, Needle Free Devices, Drug Administration, Drug Delivery

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APPLICATION OF QUALITY BY DESIGN (QbD) CONCEPT IN THE DEVELOPMENT OF CO-PROCESSED MCC PELLETS

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Abstract: Quality by Design (QbD) is a systematic approach to development that begins with predefined objectives and emphasizes product and process understanding and process control, based on sound science and quality risk management [1, 2]. Co-processing of excipient is a less expensive approach to obtain excipients of superior properties and multifunctional activities [3]. Microcrystalline cellulose (MCC) is the most widely used excipient for the production of pellets by extrusion-spheronization due to plasticity and cohesiveness of the wet mass. However, it causes slow release of poorly water- soluble drugs [4, 5]. The objective of present study was to develop co-processed MCC core pellet by applying principle of QbD. Co-processed excipient core pellets were prepared by extrusion spheronization technique and drug was coated onto it in a fluidized bed processor. Quality Target Product Profile (QTPP) and Critical Quality Attributes (CQA) for core and coated pellets were identified and evaluated. Ishikawa diagram was plotted for risk analysis. The first set of experiments was organized according to Plackett–Burman design, followed by the Box Behnken design. Finally, the control space was established within which the desired quality of the pellets can be obtained. Product development using QbD approach can definitely assured quality in the product.

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Synthesis, Characterization and biological evaluation of benzothiazolyl-triazolyl-chromenone derivatives

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Abstract: The greatest challenge confronting malaria and tuberculosis chemotherapies is the growing incidence of drug resistance against clinically established drugs. The causative agents of these diseases, Plasmodium falciparum and Mycobacterium tuberculosis, are a major global problem with millions of deaths being reported every year. This combined with the emergence of drug resistance necessitated increased efforts to search for new chemical compounds with novel modes of action. Similarly, the diminishing efficacy of currently used anti-TB & antimalarial drugs coupled with the emergence of resistant strains compliment the need to discover novel drugs. Thus, in demonstration, as part of our drug discovery programme the synthesis of an exploratory library of the hybrids modelled on the chromenone, benzothiazole and triazole moieties were undertaken.A series of substituted benzothiazolyl-1,2,4-triazolyl-chromenone derivatives were synthesized. Structures and purity of these compounds were confirmed using IR, ^{1}H & ^{13}C-NMR and elemental analysis. Also, all the synthesized compounds were screened *in vitro* for their antibacterial activity, antifungal activity against selected pathogens. Furthermore, the antitubercular & antimalarial activity of these newly synthesized compounds was also evaluated.

Keywords: Benzothiazoles, Triazoles, *2H*-chromen-2-one, Drug resistance, Antitubercular, Antimalarial, Pharmacophore hybridization.

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Influence of Poloxamer on Losartan loaded Nanoparticles

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Abstract: A novel controlled release system of Losartan loaded Poly (ε-caprolactone) (PCL)/Poloxamer F68 blend Nanoparticles is reported in the present research work. Losartan-loaded PCL/Poloxomer F68 Nanoparticles were prepared by modified water-in-oil in-water (w/o/w) double emulsion solvent evaporation technique using different formulation variables such as concentrations of drug, emulsifier and polymeric blend. The influence of these variables on surface morphology, particle size distribution, encapsulation efficiency, and *in vitro* release behaviour were examined. From the result it has been reviled that concentration of Poloxamer affects the porosity and drug release. The results also indicate that the prepared nanoparticulate system seems to be promising tools for controlled drug release in future.

Keywords: Losartan, Poly (ε-caprolactone). Poloxomer F68, Nanoparticles, Modified solvent evaporation/extraction technique, Release kinetic models

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Design, Synthesis and biological evaluation of β-amino carbonyl compounds catalyzed by a novel catalyst under solvent-free conditions

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Abstract: Solvent-free reactions are of great importance in organic synthesis as these reduce the environmental pollution, save energy and bring down the handling costs due to simplification of work up technique. Herein, salt, pyridinium trifluoro/trichloro acetate with weak acidic character has been synthesized and subsequently used as the catalyst for one-pot three-component Mannich reaction under solvent-free condition at room temperature. All the newly synthesized β-Amino carbonyl compounds were obtained in reasonable yields. The products could be separated from the catalyst simply via washing with water and after removing water, the catalyst could be recycled and reused. Structures and purity of these compounds were confirmed by elemental, IR, NMR (^{1}H & ^{13}C) spectral analysis. Newly synthesized compounds were also tested for their *in vitro* anti-tubercular activity against *Mycobacterium tuberculosis H37Rv*, *in vitro* antibacterial activity against selected pathogens viz. *E. Coli, P. Aeruginosa, Kl. Pneumoniae, S. Typhi, S. Aureus, S. Pyogenus, B. Subtilis* and antifungal activity against *C. Albicans, A. Niger, A. Clavatus strains.*

Keywords: Solvent Free Condition, Mannich Reaction, Pyridinium trifluoroacetate, β-Amino carbonyl compounds, anti-tubercular activity, antibacterial and antifungal activity.

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Design, Synthesis and Evaluation of 2-[(Substituted aryl/heteroarylamino)-methyl]-3-[*N*-isonicotinamide-yl]-quinazoline-4-one Derivatives as Potent Antimicrobial and Antitubercular Agents

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Abstract: Novel heterocyclic systems, viz. 2-[substituted-4-phenyl-thiazol-2-yl-aminomethyl]-3-[*N*-isonicotinamide-yl]-quinazoline-4-one **(3a-l)** and 2-[substituted-benzothiazol-2-yl-aminomethyl]-3-[*N*-isonicotinamide-yl]-quinazoline-4-one **(5a-l)** have been synthesized from the key intermediate 2-chloromethyl-3-(*N*-isonicotinamide-yl)-4*H*-quinazolinone **(1)**. Structural characterization was done using IR, ^{1}H & ^{13}C-NMR and elemental analysis. Also, all the synthesized compounds were screened *in vitro* for their antibacterial activity against gram negative organism, gram positive organism and antifungal activity against selected fungicidal pathogens. Furthermore, the antitubercular activity of these newly synthesized compounds was also evaluated against *Mycobacteria tuberculosis H37Rv*. Some of them are showing promising antimicrobial and antitubercular activity.

Keywords: Quinazoline-4-one, Heteroaromatic compounds, Antitubercular, Antibacterial, Antifungal activity

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A Pulsatile Drug Delivery System: A novel technology

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Abstract: Current research in Drug delivery devices, Pulsatile drug delivery system is most interesting time and site-specific system. Pulsatile drug delivery system provides a promising approach towards chronic disease like Asthma, Peptic Ulcer, CV disease, Arthritis & Hypercholesterolemia by delivering drug at right time, right place and in a right amount. [1] Various design strategies proposed including time controlling, stimuli induced, externally regulated & multiparticulate formulation. Different system like capsular system, osmotic system, single & multiple unit system based on use of soluble/erodible polymer coating & use of rupturable membrane have been dealt with in this article. These systems are beneficial for drug having Chronopharmacological behaviour where night time dosing is required. Traditionally, Drugs are released in an immediate or extended manner, where pulsatile drug released rapidly after a well-defined lag-time to achieve desired therapeutic effect & reducing side effect, so patient compliance can be obtained along with lowering dose frequency. Current review discussed reasons for development of pulsatile drug delivery system, types of disease in which pulsatile release required, classification, advantages, limitations, and polymers used in pulsatile drug delivery system.

Keywords: PDDS, Chronic Disease, rupturable membrane, Lag-time.

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Synthesis, Characterization and Biological Evaluation of Some Isoxazole Based Chromeno Pyrimidine Derivatives

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

Keywords: chromenopyrimidine, isoxazole, antimicrobial

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P-144

"Synthesis, Characterization and Physico-Chemical properties of Homopolyesters based on *s*-triazine ring"

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Abstract: Various homopolyesters have been synthesized byhigh temperature polycondensation of 2-(*N*-diphenylamine)-4,6 bis(phenoxy-4'-carbonylchloride)-*s*-triazine with various diols such as: Bisphenol-A, Bisphenol-C, Catechol, Resorcinol, Hydroquinone, Ethylene Glycol, Diethylene Glycol, Triethylene Glycol and Phenolphthalein. All the synthesized polyesters have been characterized bysolubility, density, viscosity IR spectra, ^{1}H NMR spectra and Thermo Gravimetric Analysis.

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SYNTHESIS AND CHARACTERIZATION OF ACID DYES BASED ON 2,2'-METHYLENE BIS(5-AMINO BENZOIC ACID) AND THEIR APPLICATION ON VARIOUS FIBERS

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Abstract: A series of acid dyes has been synthesised by coupling of tetrazotized 2,2'-methylene bis (5-aminobenzoic acid) and coupling with various pyrazolone coupling components. The structure elucidation of all dyes was established by UV, IR and ^{1}H NMR spectra. The dyeing performance of all these dyes on wool and silk has been studied. The dyed fabric showed moderate to very good light fastness and good to excellent washing and rubbing fastness properties.

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Synthesis and Biological Evaluation of some Schiff Base Derivatives having Benzothiazole moiety

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Abstract: A series of Schiff base derivatives of 6,6'-methylene bis (N-substituted benzylidene-4,7-dimethylbenzo[d]thiazol-2-amine) has been synthesized by condensing benzothiazole derivative with various aromatic aldehydes. The synthesized compounds were characterized and evaluated for antimicrobial activities. The newly synthesized compounds were tested against representatives of gram-positive and gram- negative bacteria. A number of benzothiazole derivatives have exhibited interesting biological activities [1-2].

Keywords: Benzothiazole, aldehydes, antimicobial

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P-147

Determination of Biological activities of newly synthesized Pyrazolone based Formyl derivatives and Schiff bases

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Abstract: Among the various properties of chemical compounds, pharmacological/biological activity plays a crucial role since it suggests uses of the compounds in the medical applications; however chemical compounds may also show some adverse and toxic effects which may prevent their use in medical practice [1, 4]. In medicine, Pyrazolone are well known for their wide medicinal applications like, analgesic, anti-inflammatory, antipyretic, antiarrhythmic, tranquilizing, muscle relaxing, psycho analeptic, and anticonvulsant, monoamineoxidase inhibiting, antidiabetic and antibacterial activities. In pharmacology, biological activity or pharmacological activity describes the beneficial effects of a drug on living matter, this is exploited in drug development to increase the concentration of a compound in the blood by adjusting the pK_i of an ionizable group [2, 5]. We designed pyrazolone base compounds [3] and characterized by spectroscopic and crystallography and evaluation its antioxidant as well as it biological applicability by experimenting them with certain strains of Gram Positive and Gram Negative bacteria's. We performed antioxidant activity with Ferric reducing antioxidant power assay (FRAP) and 2,2 diphenyl-1-(2,4,6-trinitrophenyl hydrazyl) (DPPH), all the compounds show good antioxidant activity as well as biological activities within the range of 12% to 81% in comparison with Vitamin C as standards and streptomycin respectively for reference. So our synthesized chemical compounds could be ideal antioxidant agent, antibacterial as well as antifungal with ability of slowing or preventing the oxidation of other molecules.

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P-148

Synthesis of some new bioactive heterocyclic compounds

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Abstract: 1-aryl-4-[5-chloro-3-(2,4-dichloro-5-fluorophenyl)-1H-pyrazol-4-yl]azitidin-2-one **1** and 2-[5-chloro-3-(2,4-dichloro-5-fluorophenyl)-1H-pyrazol-4-yl]-3-aryl-1,3-thiazolidin-4-one **2** have been synthesized by reaction of N-{[3-(2,4-dichloro-5-fluorophenyl)-1H-pyrazol-4-yl] methylene}aniline with chloro acetylchloride and mercapto acetic acid respectively.

P-149

Synthesis, Characterization of Schiff bases with transition metals and its remarkable study of human anti-breast cancer cell lines.

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Abstract: Schiff bases play an important role as ligands in metal coordination chemistry even after almost a century since their discovery. Modern chemists still prepare Schiff base ligands are considered as "privileged ligands" They were also reported to possess, cytotoxicity[1], anticonvulsant[2], anticancer[3], and catalysis[5],

A series of novel compounds whose structures are Schiff base based skeleton have been synthesized and characterized. These Schiff bases were derived from aryl aldehydes and 5-(3-Bromo-4-methoxyphenyl)-4-{[substitutedphenylmethylidene]amino}-4H-1,2,4-triazole-3-thiol . Most of the reactions have been successfully applied and used, as many of the synthesized compounds exhibit interesting biological activity in the fields. The structures of synthesized compounds were established on the basis of ^{1}H NMR, FTIR spectroscopy as well as by X-ray diffraction. The compounds were evaluated for in vitro anticancer activity. The most active compounds from the series displayed GI50 value equal to doxorubicin against the strain of human breast cancer cell line MCF-7.

Keywords: Schiff bases, transition metal , anti-cancer activity.

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P-150

Selective isomers for pharmaceutical application of drugs.

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Abstract: Selection and administration of more effective less toxic and lower side effect of drugs is challenging task for physician. In recent, importance of stereochemistry in drugs action is gaining great attention in medical practice. Now a days more than 50% of the drugs currently in use as a chiral compounds, and near 90% of drugs are marked as recemates consisting an equimolar mixture of two enentiomers. Chiral drug exhibit marked difference in biological activities, live pharmacology, toxicology, pharmaceuticals metabolism etc. In our article we elaborate selective single enentiomer is more selective for biological target, improved therapeutical action and better pharmaceutical action with less side effect then mixture of isomers.

P-151

Prevalence of multi drug resistant coliforms inmunicipal sewage.

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Abstract: Aquatic systemsare being polluted and enteric pathogens are frequently found in it. Due to the indiscriminate usage of antibiotics, enteric pathogens are known to develop multidrug resistance that poses a serious note to human health. Coliforms are a group of bacteria that are known to occur in aquatic sources and are traditionally used for water quality estimation. The application of antibiotics against bacteria are known to become ineffective after some time. It is of pivotal importance for us to identify an alternate(preferably an environment friendly) or new sourcesto restrict MDR coliforms in their natural environments.

A master's thesis project has been initiated to isolate and enumerate various multidrug resistant (MDR) coliforms from aquatic sources, especially from municipal sewage treatment sources of South Gujarat region and to test their susceptibility to plant extracts. Water samples before and after the treatment, from three different placesVapi, Navsari and Surat were collected and their physiochemical properties were recorded. MDR coliforms wereenumerated by cultivation based methods followed by their isolation. Preliminary results indicate four morphologically different (based upon colony morphology) organisms were isolated.They were also tested for their tolerance towards heavy metals (Ag, Cu, Fe and Zn). Molecular identification of isolated bacteria is still in progress.The isolated MDR coliforms will be tested against various plant extracts and their mixtures for MDR coliforms susceptibility.

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Pharmacophores Hybridization: Design & Evaluation of Some Newer Triazolyl-Thiol Analogous Bearing Diphenyl Ether Nucleus

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Abstract: Certain small heterocyclic molecules known as pharmacophores are biologically active and medicinally useful molecules. In earlier work structure design studies resulted that the diphenyl ether, triclosan[1] is a potent inhibitor of ENR's from many organisms including *Escherichia coli* and *Plasmodium falciparium*[2,3] Using structure-based drug design we developed a series bearing a diphenyl ethers nucleus.[4-6]A novel series of diphenylether based namely (Z)-5-((substituted amino phenyl) methyl)-4-(3-phenoxybenzylideneamino)-4*H*-1,2,4-triazole-3-thiol(6a-j) has been synthesized by condensation of m-phenoxybenzaldehyde with 4-amino-5(substituted amino phenyl)methyl)-4H-1,2,4-triazol-3-thiol(6a-j) which synthesized from the parent intermediates(1a-j). These newly synthesized compounds were characterized by NMR, IR spectral study and were evaluated for their antimicrobial activity compared to standard drugs.

Keywords: diphenylether, triazolylthiol, antimicrobial activity.

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Nitrogen-Oxygen Containing Heterocyclic Synthesis via Microwave-Conventional Blend Approach and their Biological Response

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Abstract: Pyridine, Pyrimidine[1] and Oxadiazole[2-3] derivatives which can facilitate the development of more potent and effective antimicrobial agents. For that we have synthesized N-(5-(4-(4-substituted phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidin-5-yl)-1,3,4-oxadiazol-2-yl)-2-((3-cyano-4-(3,4-dichlorophenyl)-6-(4-hydroxy-3-methoxyphenyl)pyridin-2-yl)amino)acetamide **1a-m** via microwave synthesis. Multi component Beginelli[5-6] reaction followed by oxidative cyclization to generate 1,3,4-oxadiazole and condensed with amino pyridine using microwave and conventional blend concept. The structures of newly synthesized derivatives were assigned by spectral and analytical data and they were evaluated for their biological response against bacterial and fungal species where they had showed promising antibacterial and antifungal activities.

Keywords: Pyridine, Pyrimidine, Oxadiazole, Microwave-Conventional blend, antibacterial and antifungal activities

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P-154

Thermal and Physicochemical studies of polymers derived from s-Triazine

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Polyesters containing s-triazine in the main chain are known for their high transition temperature and thermal stability. The choice of this heterocycle is based on its high thermal stability derived from its molecular symmetry and aromaticity. Ten polyesters have been synthesised by high temperature polycondensation of substituted s-triazine with different diols: bisphenol-A, hydroquinone, catechol, resorcinol, ethylene glycol, diethylene glycol, phenolphthalein, 1,4-dihydroxy anthraquinone , 1,5-dihydroxyanthraquinone, 1,8-dihydroxy anthraquinone. The synthesised polyesters were characterised by various techniques like FTIR, NMR, viscosity and fluorescence. The relative solubility of these polyester samples were determined in a variety of solvents. Thermal stability was studied by TGA and DTA techniques. The obtained polyesters possess high thermal stability with good solubility in organic solvents.

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Synthesis, characterization and dyeing performance of compounds based on nitro thiazole

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Abstract: N^4-(5-nitrothiazol-2-yl) thiazole-2, 4-diamine derivatives have been synthesized by the reaction of 2-amino 5-nitro thiazole and chloroacetylchloride with suitable solvent then cyclized with thiourea at reflux temperature in methanol to yield N^4-(5-nitrothiazol-2-yl) thiazole-2, 4-diamine which was diazotized and coupled with various couplers 3^{o}amines to give new series of disperse dyes **(D_1-D_{14})**. All the compounds were characterized by their percentage yield, melting point, elemental analysis, UV spectra, IR spectra, NMR spectra and dyeing performance on polyester fabric was assessed. The fastness properties of dyes were evaluated using standard methods. All the synthesized dyes gave moderate to excellent fastness properties on polyester fabric which gave purple, pink, brown to orange hue. Computer color matching properties was assessed.

Keywords: 2-amino 5-nitro thiazole, chloroaecetyl chloride, dyeing, 3^{o}amines, fastness properties

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Synthesis of bifunctional reactive dyes and their application on various fibres

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Abstract: A series of bifunctional reactive dyes has been synthesized by coupling of tetrazotized 4,4'-methylene bis(2-methoxy aniline) with various 2-(4-amino phenyl sulphonyl) ethyl hydrogen sulphato cyanurated coupling components such as H-acid, Gamma acid, J-acid, N-Methyl J-acid, N-Phenyl J-acid, Chicago acid, S-acid, K-acid, Bronner acid, Peri acid, Laurent acid, Koch acid, Naphthionic acid and Tobias acid. They were characterized by nitrogen elemental analysis, IR and ^{1}HNMR spectra. The dyeing performance of all these dyes on wool, silk and cotton fibres gave fair to good light fastness, good to excellent fastness to washing and rubbing fastness.

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Synthesis of monoazo reactive dyes and their application on various fibres

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Abstract: A series of monoazo reactive dyes has been synthesized by coupling of diazotized aniline with various 4-(4-methoxyphenyl)-6-phenylpyrimidin-2-amino cyanurated coupling components such as H-acid, Gamma acid, J-acid, S-acid, Koch acid, Bronner acid, Tobias acid, Cleve acid, Peri acid and Laurant acid. They were characterized by nitrogen elemental analysis, IR and ^{1}HNMR spectra. The dyeing performance of all these dyes on wool, silk and cotton fibres gave fair to good light fastness, good to excellent fastness to washing and rubbing fastness.

P-158

"Synthesis and Physico-Chemical properties of 2-(N-piperidino)-4,6-bis(2-naphthoxy, 6-carbonylchloride)-s-triazine based Copolyesters

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Abstract: Variouscopolyesters have been synthesized byhigh temperature polycondensation of 2-(*N*-piperidino)-4,6-bis(2-naphthoxy, 6-carbonylchloride)-*s*-triazine [PNCCT] with various mixture of diols. [1,2] All the synthesized polyesters have been characterized bysolubility, density, viscosity IR spectra, ^{1}H NMR spectra and Thermo Gravimetric Analysis.

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P-159

Synthesis and characterization of Cold Brand Reactive Dyes based on 4,4'-methylene bis-orthonilic acid derivative and their dyeing performance on various fibres

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Abstract: A series of cold brand reactive dyes has been synthesized by coupling of tetrazotized 4,4'-methylene bis-orthonilic acid with various cyanurated coupling components[1,2].The synthesized compounds were characterized by the UV-Visible, IR&^{1}HNMR spectroscopy. Their dyeing performance on silk, wool and cotton has been assessed. The percentage dye bath exhaustion on different fibres was reasonably good and acceptable. The dyed fibres showed moderate to very good fastness to light, washing and rubbing.

Keywords: 4,4'-methylene bis-orthonilic acid, cyanurated coupling components, dyeing performance.

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A newer series of Reactive Dyes based on 4,4'-methylene bis-2,5-dimethylaniline derivative: Synthesis, characterization and applications

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Abstract: A series of hot brand reactive dyes has been synthesized by coupling of tetrazotized 4,4'-methylene bis-2,5-dimethylaniline with various cyanurated coupling components[1-3].The synthesized compounds were characterized by the UV-Visible, IR &^{1}HNMR spectroscopy. Their dyeing applications on silk, wool and cotton have been assessed. The percentage dye bath exhaustion on different fibres was reasonably good and acceptable. The dyed fibres showed good fastness to light, washing and rubbing.

Keywords: 4,4'-methylene bis-2,5-dimethylaniline, cyanurated coupling components

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Microwave Assisted Synthesis of Fly Ash Supported Nickel Oxide Nanoparticles

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The present study illustrates the synthesis of fly ash supported nickel oxide nanoparticles as cost effective catalyst for generation of reactive oxygen species for waste water treatment. A novel microwave assisted synthesis is described in which urea is used as fuel and nickel nitrate as oxidizer. Fly ash is chemically activated prior to being used as support material for catalyst synthesis. The experimental details of thermal and chemical activation of fly ash are reported which modified neutral surface of fly ash into basic surface responsible for intensified bonding and dispersion of NiO nanoparticles over fly ash surface. The physico-chemical and morphological characterization of fly ash, chemically activated fly ash and fly ash supported nickel oxide have been carried out using AAS, XRD, FT-IR, SEM-EDX techniques. To evaluate the catalytic activity decomposition reactions of hydrogen peroxide have been selected, effects of different parameters such as pH, calcination temperature, nature of catalyst etc., have been checked to optimize the catalytic reaction.

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Isolation and Characterization of Mannanase Producing Bacteria from Dahalia and Sugarcane Rhizosphere

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Abstract: Mannanase is an endohydrolase, which is a member of glycosyl hydrolase families 5 (GH5) and 26-β (GH26-β). As an endohydrolase it hydrolyzesthe internal bonds of a mannan containing polysaccharide [1]. The potential application of Mannanase in production of manno-oligosaccharides, which are utilized selectively by intestinal *Bifidiobacterium* species and also this enzyme,is used in food, feed, textiles and Pharmaceutical industries [2]. The present study aims to isolate and screen high mannanase producing bacteria from the rhizosphere of Dhalia and sugarcane plants. A total of 58 bacillus strains were isolated from rhizospheres ofDhalia and sugarcane plants,planted at nursery and agriculture field of Bardoli, Gujarat, India. These isolates were screened for the ability to hydrolyze copra meal, locust bean gum and indirect assay to estimate the release of reducing sugar by 3,5-Dinitrosalicylic acid methods.From theprimary screening methods it revealed that 9 bacillus strains were capable to produce extracellular mannanase.

Keywords: Biochemistry, Molecular Biology and Cell Biology Research

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P-163

Synthesis and Characterization of newer Sulfonamide derivatives having Sydnone and Benzothiazole moieties as an antimicrobial agents

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Abstract: One of the distinct area of heterocyclic compounds is a class of mesoionic compound. Sydnones are very important members of this class. A series of sulphonamide derivatives has been synthesized by condensing 4-(chlorosulfonyl)-3-(4-methoxyphenyl)sydnone[1-2] with various benzothiazoles[3]. The synthesized compounds were characterised and evaluated for antimicrobial activities. The newly synthesized compounds were screened against representatives of gram-positive and gram-negative bacteria. All the synthesized compounds were characterized by elemental analysis, IR and ^{1}H NMR spectra.

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P-164

Synthesis and dyeing assessment of tetra azo acid dyes derived from 4,4'-(propane-2,2-diyl)bis(2-methyl-4,1phenylene)bis (3-aminobenzenesulfonate)

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Abstract: 4,4'-(propane-2,2-diyl)bis(2-methyl-4,1-phenylene)bis(3-aminobenzenesulfonate) was synthesized by reduction of condense product of Bisphenol C and m-nitrobenzenesulfonyl chloride. The compound was used as a bifunctional middle component in the preparation of tetra azo acid dyes. This di amino compound was tetra azotized and coupled with naphthalene based acid coupling component to give various tetra azo acid dyes. The obtained dyes were characterized by spectroscopic technique (UV-vis., IR, NMR) and the dyeing assessment of all dyes was evaluated on wool, silk and nylon fabrics. These dyes gave red, brown, violet, and pink shades on each fibers with good to very good fastness properties. The percentage dye bath exhaustion and fixation was also been studied.

Keywords: Bisphenol C, m-nitrobenzenesulfonyl chloride, Tetra azo acid dyes, Fastness properties

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Larvicidal activity of essential-oil-loaded nanoemulsions against filariasis vector

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Abstract: Mosquitoes play predominant role as vectors of pathogens causing dreadful diseases like malaria, dengue fever, yellow fever, filariasis, chikungunya and japanese encephalitis [1]. *Culex quinquefasciatus* is one of the important vectors of filarial parasite *Wuchereria bancrofti* [2]. Potential risks associated with the use of toxic synthetic pesticides lead to an abrupt and urgent necessity to develop ecofriendly and more efficient alternative to replace these synthetic pesticides [3]. Essential oils are bio-based pesticides with significant larvicidal properties [4]. Nanoemulsions are dispersions of oil and water with droplet size in the range of 10–100 nm [5]. Plant essential oil based nanoemulsion was formulated by ultrasound cavitation method. Droplet size of optimized nanoemulsion was 24 nm. Formulated nanoemulsion demonstrated dose and time dependent larvicidal activity against *Culex quinquefasciatus.* Complete loss of larval viability was observed within in 6 hr of interaction with 100 ppm nanoemulsion, whereas it took 18 hr and 24 hr when interacted with 75 ppm and 50 ppm of nanoemulsion respectively. Formulated nanoemulsion was observed to be an efficient larvicide against *Culex quinquefasciatus* even at very low concentration of 5 ppm. After 24 hr of interaction with 5 ppm of nanoemulsion, 50 % larva mortality was observed. Histological staining confirmed the damage caused by nanoemulsion treatment. Larvicidal activity of the plant essential oil nanoemulsion can be attributed to the lower droplet size of nanoemulsion and the bioactive component in the essential oil. Further, this nanoemulsion formulation can be used for mosquito vector control.

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SYNTHESIS AND CHARACTERIZATION OF Mg-Al-CO_3 LAYERED DOUBLE HYDROXIDES

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In the present work Mg-Al-CO_3 LDHwas prepared, using ammonium carbonate, at variable as well as constant pH along with different Mg:Al ratio. Different instrumental techniques such as X-ray diffraction, FTIR and scanning electron microscope (SEM), BET surface area analyzer were used to characterize the samples. The effect of different synthetic parameters such as addition temperature, agitation, drying temperature, and pH were also studied.Surface area of Mg-Al-CO_3 LDH for Mg:Al ratio 2:1, precipitated at constant pH, was observed to be maximum (84 m^2/g). It was observed that crystallinity of Mg-Al-CO_3 LDH samples decreases with increasing the Al content in the sample. Mg-Al-CO_3 LDHs were obtained with diverse morphology, because of uncontrolled precipitation. Addition and drying temperature shows significant effect on the crystallinity of the samples. It was observed that addition of solution at room temperature slightly favors the crystallinity and drying of LDH sample at room temperature enhanced the crystallinity of the sample as compared to oven drying at 110 ^{0}C.

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2,4-dihydroxy-5-bromo-(2'methyl) propiophenonethiosemicarbazone [DHBMPT] as an Analytical Reagent: Studies on Co(II) chelate

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2,4-dihydroxy-5-bromo-(2'methyl)propiophenonethiosemicarbazone [DHBMPT] has been used for the spectrophtometric determination of Co(II) at pH = 9.0. Job's method of continuous variation and Yoe and Jones Mole ratio method show metal: ligand ratio in the complex to be 1:2.The molar absorptivity of complex at 410 nm was found to be 2.49 x 10^3lit. $mol^{-1}.cm^{-1}$ and Sandell's sensitivity was found to be *0.0237*µg/cm^2.The stability constant determined spectrophotometrically is found to be *2.73 x* $10^{10}$and Gibb's free energy change for complex formation reaction is calculated to be -*14.324* k cal /mole. The Beer law is obeyed up to 9.43ppm of Co (II) ion at 410nm. From TGA studies, the energy of activation for the decomposition stepshas been calculated. The reagent has been satisfactorily applied for the determination of Cobalt in Cobalt metal sample.

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Impact of pollution on seawater, sediments and Mangroves; Physico-chemical & Biological parameter, Nutrient and Heavy metals in South Gujarat estuarine regions

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Abstract: The rapid industrialization and anthropogenic activities along the estuarine system and the coastal areas have brought aconsiderable decline in the water quality of the estuaries.Uncontrolled discharges of domestic wastes and industrial effluents have affected the south Gujarat estuarine regions. Seawater, sediments, and mangroves samples were collected from eight different sampling points in south Gujarat coasts to study the physico-chemical characteristics. Determination of some important physico-chemical parameters of seawater and sediments of south Gujarat estuary at South Gujarat was carried out. The physico-chemical parameters such as pH, conductivity, salinity, turbidity, inorganic phosphate, nitrite, nitrate, total nitrogen, dissolved oxygen, biological oxygen demand, heavy metals, phenol and organic matter were determined for entire south Gujarat area. Our study showed correlation between salinity and conductivity.Analysis of chlorophyll, malondialdehyde and heavy metals in mangrove samples was done by standard protocols. The study exemplified the fact that the south Gujarat mangrove ecosystem is not agood state of health.The present study demonstrated that the concentration of lead, chromium, and nickel in seawater and sediments beyond the tolerance limits. The presence of high concentration of lead and chromium yields harmful effect on marine, coastalecosystem and to that of human life.

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Design, Synthesis, Characterization and antimicrobial screening of some benzimidazole based pyrazole derivatives

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Abstract: The smoldering need of great importance for chemist is to synthesize pharmaceutical molecules with more prominent resistance than the current scaffolds. In continuation to this, the present work deals with the synthesis and antimicrobial activity of novel series of 1-(3-(1*H*-benzoimidazol-2-yl)-5-phenyl-4, 5-dihydro-1*H*-pyrazol-1-yl)-2-(naphthalen-1-yloxy) ethanone. All the newly synthesized compounds were screened for *in vitro* antibacterial activity against *Escherichia coli, Pseudomonas aeruginosa, Staphylococcus aureus and Streptococcus pyogenes* and for antifungal activity against *Candida albicans, Aspergillus Niger* and *Aspergillus clavatus* by using serial broth dilution method. The structures of the compounds were elucidated by IR, ^{1}H-NMR, ^{13}C-NMR and Mass spectra.

P-170

Impounding of Aromatic compounds using Barium incorporated and improved Si/Al ratio Microwave synthesized Bagasse fly ash based Zeolitic materials

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Abstract: Water pollution by aromatic compounds has been given great attention now days. Strict environmental permissible limit for pollutants are familiar in many countries. In some developing countries, how to deal with large volume of wastewater containing toxic organic pollutants is a pressing environmental issue. Organic compounds such as p-nitroaniline nitrobenzene and aniline are important intermediates to produce perfumes, synthetic resins, drugs dyes, fuel additives, antioxidants, and pesticides etc as a result; the aromatic compounds containing wastewater has been introduced into water bodies. Contaminated water bodies cause adverse effect on the environment and human health. Adsorption is the best remedy to impound pollutants from the solutions. Thus microwave synthesized, Barium impregnated (EMZBFA-Ba) and enhanced Si/Al ratio (EMZBFA-30-Ba) has been synthesized from Bagasse Fly Ash (BFA) for sorption of the aromatic pollutants. The sorbents were characterized using PXRD, XRF, FTIR, SEM, TGA, BET and BJH techniques. The operational parameters like pH, agitation time, initial sorbate concentration, adsorbent dose and temperature have been studied. Sorbates removal efficiency observed at optimized parameters had average sorption capacity of para-nitroaniline (qe): 24.50 mg/g, 30.10 mg/g, and 33.80 mg/g, nitrobenzene (qe):27.56 mg/g, 36.12 mg/g, and 39.26 mg/g, aniline (qe): 39.06 mg/g, 45.02 mg/g and 48.59 mg/g for BFA, EMZBFA-Ba, with EMZBFA-30-Ba respectively Freundlich isotherem model best fitted for sorption process while the kinetic studies show pseudo second order rate of sorption. Intraparticle diffusion and surface adsorption were suitable for taking out of p-nitroaniline nitrobenzene and aniline from the solution.

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Statistical modelling of Box Behnken Design on Ortho-chlorophenol removal by magnetic zeolitic composites transformed from Bagasse Fly Ash

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Abstract: The present study focuses on the sorption behaviour of Ortho chlorophenol (OCP) onto magnetic zeolitic composites derived from agricultural waste Bagasse Fly Ash (BFA). The sorption of OCP was improved by modifying virgin BFA by electrolyte supported microwave hydrothermal treatment (MZBFA) and magnetic modification (MMZBFA). The synthesized adsorbents were characterized by some instrumental techniques (XRF, PXRD, SEM, FTIR and TGA). The adsorption process was optimized under four different variables like: pH (4-7), agitation time (30-120 min), initial adsorbate concentration (50-150 mg L^{-1}), adsorbent dosage (1-4 g L^{-1}) based on Box- Behnken Design (BBD) with Response Surface Methodology (RSM). The highest predicted adsorption capacities at pH 7 with 1 g L^{-1} adsorbent dose for MZBFA and MMZBFA were 29.95 mg g^{-1} and 31.94 mg g^{-1} for agitation time of 75 min and 120 min, initial adsorbate concentration was 150 mg g^{-1} and 100 mg g^{-1} respectively which were approximated with laboratory results. The isotherm data and kinetic data were best described by Langmuir model and pseudo second order model respectively. The adsorbents are stable after three cyclic runs when regenerated with 0.1 M NaOH solution.

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Synthesis of surface modified zeolitic materials by microwave irradiation of power station thermal waste for amputation of p-Nitrophenol from aqueous solution

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Abstract: The purpose of this work was to synthesize low cost adsorbent from power station solid waste-coal fly ash (CFA), by electrolyte treated (MZCFA) and surfactant modified (SMZCFA) using microwave irradiation techniques. The raw material and synthesized adsorbents have been characterized by instrumental techniques like PXRD, XRF, FT-IR, SEM and TGA. The raw coal fly ash and synthesized adsorbent has been utilized for sorption of p-Nitrophenol from aqueous solution. To investigate sorption proficiency equilibrium time, pH, concentration, dose and temperature variable have been studied. Thermodynamic variables have been assumed to know the feasibility of sorption processes. Batch studies followed sorption capacity order as SMZCFA (38.24 mg g^{-1}) > MZCFA (33.85 mg g^{-1}) > CFA (20.55 mg g^{-1}). Adsorption isotherm and kinetic studies have been performed out of which Langmuir isotherm (R^2=0.999) and Pseudo-second-order (R^2=0.998) are best fitted, respectively. Column dynamics have been investigated for each system. Regeneration studies have been adapted by using 0.5M HCl and NaOH solutions.

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SYNTHESIS OF HETEROCYCLIC COMPOUND BEARING s–TRIAZINE MOIETIES AND THEIR ANTIMICROBIAL EVALUATION

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Abstract: Some new substituted 1,3,5 triazine with primary amine were synthesized and evaluated for their *in vitro* antimicrobial activity against Gram positive and Gram negative strains using a microdilution procedure. Synthesized compounds prove to be effective with MIC (mg ml^{-1}), among them some of compoundshowed excellent activity against a panel of microorganisms. The newly synthesized compounds were characterized using **IR**, ^{1}**H-NMR**.

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Synthesis and liquid crystalline investigation of chiral 6-alkoxy-2-naphathoic acid derivatives

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Abstract: A two new series of materials with a chiral fragment derived from ((*S*)-(─)-2-methyl-1-butanol and 6-alkoxy-2-naphathoic acid as the molecular core was synthesized and investigated. All thehomologues exhibited enantiotropic mesomorphism. chiral smectic C (SmC*), smectic A (SmA) and chiral nematic (N*) phases were observed in different homologues. All the compounds were characterized by spectroscopic andelemental analysis. Thermal investigations and mesophase characterizations for all the compounds were carried out by the combination of DSC and POM analysis. The effects of the central linkage and various terminal normal alkyl chains with its structurally relatedcompounds have been discussed.

Keywords: calamitic liquid crystal; chiral smectic SmC* phase; chiral nematic N* phase; cinnamate; ester; smectic A phase

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Synthesis and Characterization of some cyanurated polyesters

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Abstract: Some polyester have been synthesized using condensation of oxyalkyl derivative of cyanuric chloride and 6-hydroxy-2-naphthoic acid. Resultant compounds were treated with epoxy resins, after that compounds were polymerized using acryloyl chloride. All the compounds were characterized by spectroscopic technique like IR and ^{1}H NMR. The physical properties of synthesized compounds were measured by solubility, density, viscosity, TGA analysis.

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STUDIES ON PHYTOCHEMICAL INVESTIGATION AND ANTIMICROBIAL ACTIVITIES OF ENDOPHYTIC FUNGI ISOLATED FROM SOME IMPORTANT MEDICINAL PLANTS

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Abstract: Endophytic fungi and bacteria which live within plant parts like stem, leaf and roots. These are the organisms which do not cause any harm to plant and they have been implicated in mutualism, decreased herbivory, decreased drought resistance and increased disease resistance, enhancement of plant growth. The searches for novel secondary metabolites mainly focus on the organisms that inhabit novel biotopes. Endophytes have great potential as producers of several important and novel bioactive compounds. This research mainly focuses upon phytochemical, antibacterial and antifungal activities of medicinal plants and also isolation of endophytic fungi. These isolated fungi were screened to find out bioactive compounds which these organisms produced.

Keywords: Endophytes, Phytochemical, Bioactive

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