ISCBC-NIPiCON-2020

26th ISCB INTERNATIONAL CONFERENCE (ISCBC-2020)

Jointly Organize With

5th NIRMA INSTITUTE OF PHARMACY INTERATIONAL CONFERENCE (NIPiCON-2020)

INTEGRATING CHEMICAL, BIOLOGICAL AND PHARMACEUTICAL SCIENCES FOR INNOVATIONS IN HEALTH CARE

22-24 January, 2020

Nirma University, Ahmedabad, India

ABSTRACT BOOK

Organized by:

Indian Society of Chemists & Biologists (ISCB)

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26th ISCB International Conference (ISCBC-NIPiCON-2020)

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Vice Chancellor, Gujarat Vidhyapeeth
President, ISCB

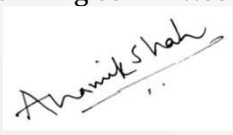
Dr. P.M.S. Chauhan
Ex. Chief Scientist and Professor,
CDRI, Lucknow
General Secretary, ISCB

Message

We are very happy to inform you that the Indian Society of Chemists and Biologists, Lucknow, India is jointly organising its **26th ISCB International Conference (ISCBC-2020)** with **5th Nirma Institute of Pharmacy International Conference (ISCBC-NIPiCON-2020)** at Nirma University, Ahmedabad, India from 22nd – 24th January, 2020.

It is a matter of great pleasure that the focal theme of the 26th International Conference of ISCB on "**Integrating Chemical, Biological and Pharmaceutical sciences for innovations in health care**". During above conference researcher are going to discuss self reliance, sustainability & affordability of pharmaceutical substances by improving process chemistry through innovation so that India can be more competitive and self reliant on Pharma products, drug intermediates & finished formulations. Scientists across the globe, especially from USA, Greece UK, France, Poland, Slovenia, Belgium, Sweden, Italy and many other countries will participate as keynote/invited speakers to address above mentioned issues. The entire conference will be addressed by more than 60 senior scientists & professors as key-note/invited speaker while it will attract more than 600 young researchers & post doctoral researchers from entire country who will take part as oral/poster presentations.

We are glad that the scientific committee is bringing out an abstracts book covering the presentations to be made during ISCBC-NIPiCON-2020. 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 9 plenary lectures, 63 invited lectures by the eminent scientists from India and abroad. 37 Oral presentations by the young researchers are scheduled. The most heartening feature of the conference is that it is being participated with a number of young scientists and Ph. D. students and presentations are schedules in three poster sessions. On behalf of ISCB we are looking for the galaxy of speakers and young participants who made this conference a memorable event. We extend our warm welcome to all National and International delegates from pharmaceutical companies, research organization, universities and academic institutes wish them very happy stay at Jaipur. Now Finally I take this opportunity to express my sincere thanks and gratitude to members and office bearers of organizing committee of 26th ISCB International Conference (ISCBC-2020).



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Wednesday, January 22, 2020

9.00 AM - 10.30 AM	**Registration**
10.30 AM - 12.00 PM	**Inaugural Session**
12.00 PM - 12.30 PM	**High Tea**

Session – I

Chairpersons: Prof. Anamik Shah and Dr. PMS Chauhan

PL-1 12.30 PM - 1.00 PM	**Nigel G. J. Richards** Department of Chemistry, Cardiff University, Cardiff, UK **Building Better Enzymes: Redesigning DNA Polymerases to Replicate Nucleobases in Expanded Genetic Alphabets**
PL-2 1.00 PM - 1.30 PM	**Christophe LEN** Chimie ParisTech, PSL Research University, CNRS, Institute of Chemistry for Life and Health Sciences, Paris, France **BATCH AND CONTINUOUS FLOW CONVERSION OF BIOMASS INTO FURAN DERIVATIVES**
1.30 PM - 2.30 PM	**Lunch**

Parallel Session – II A

Chairpersons: Prof. N.C. Desai, Dr. Vinay Tripathi and Dr. Jignasa Savjani

PL-3 2.30 PM - 3.00 PM	**Anil Kumar Singh** Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, India **New Strategies for Design and Development of Neutral andHydrophobic Extrinsic Fluorescent Probes**
IL-1 3.00 PM - 3.20 PM	**Keshav Deo** Executive Director, Almelo Private Limited, Hyderabad, India **A Dietary Supplement use as An Anti-Aging Agent**
IL-2 3.20 PM - 3.40 PM	**Shipra Chauhan** Scientist, Zeon Coperation, Kawasaki, Japan **CYCLO OLEFIN POLYMER, THE NEW AGE MATERIAL FOR MEDICAL APPLICATION BY ZEON: OUTLINE OF ZEON MEDICAL PRODUCT**
IL-3 3.40 PM - 4.00 PM	**RameshBabu Boga** BogaR Laboratories LLC, PO Box 1554, Suwanee, GA 30024, USA **Global Healthcare Challenge of Drug Resistance: Moment of Truth and Future Prospects**

IL-4 4.00 PM - 4.20 PM	**Ravindra V. Singh** Head of India R&D, Custom synthesis and Manufacturing, Merck - Living Innovation, Sigma Aldrich Chemicals Pvt Ltd, Bangalore, India **Novel Diaminoquinazolines (DAQs) as an effective inhibitor of M. Tuberculosis, and a potential drug candidate for treatment of Tuberculosis (TB)**
4.20 PM - 4.30 PM	**Tea**

Parallel Session – II B

Chairpersons: Prof. Ashok K Prasad and Dr. Vivek Vyas

IL-5 2.30 PM - 2.50 PM	**Manjunath Ghate** Director, Institute of Pharmaccy, Nirma University, Ahmedabad, India **Design, Synthesis and Biological Evaluation of Small Molecules targeting Histone Deacetylase Inhibitors (HDAC) as Anti-Cancer Agents**
IL-6 2.50 PM - 3.10 PM	**Hemant Joshi** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan, India **A Molecular Rotor Possessing a Cl-Pd-Cl "Spoke" on a Se-Pd-Se "Axle": Efficient Catalyst for Regioselective C-5Arylation of Imidazoles**
IL-7 3.10 PM - 3.30 PM	**Sivapriya Kirubakaran** Assistant Professor, Indian Institute of Technology - Gandhinagar, India **Are DDR kinases Druggable? : Our journey towards Cancer therapeutics**
IL-8 3.30 PM - 3.50 PM	**Prajwal Nandekar** Scientist, Schrodinger, India **Transforming Drug Discovery with Advanced Computational**
IL-9 3.50 PM - 4.10 PM	**Divya Vohora** Professor, Pharmacology, Faculty of Pharmacy, JamiaHamdard University, New Delhi, India **Antiepileptic Drugs and Ketogenic Diet: An Uncanny Alliance to Bone**
4.10 PM - 4.30 PM	**Tea**

Parallel Session – III A

Chairpersons: Dr. P.M.S. Chauhan and Dr. Nagja Tripathi

IL-10 4.30 PM - 4.50 PM	**Bal Ram Singh** Professor and Director, Botulinum Research Center and Institute of Advanced Sciences, North Dartmouth, MA **The Most Poisonous Poison as a Model to Reframe Biology, Chemistry, and Physics of Evolution**
IL-11 4.50 PM - 5.10 PM	**Dalip Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **Efficient and Regioselective Functionalization of Quinolones**

IL-12 5.10 PM - 5.30 PM	**Mukesh Nandave** Associate Professor, Department of Pharmacology, Delhi Pharmaceutical Sciences and Research University (DPSRU), New Delhi, India **The Role of Omics in Personalised Medicine: A Review of Outcomes in Cardiovascular Diseases**
IL-13 5.30 PM - 5.50 PM	**Ritesh Singh** Assistant Professor, Department of Chemistry, Central University of Rajasthan, Bandar Sindri, Ajmer, Rajasthan, India **Synthetic Exploration of Aza-oxyallyl Cation Towards Oxindoles and 1,4-Benzodiazepines**

Parallel Session – III B

Chairpersons: Prof. Anshu Dandia and Dr. Shital Panchal

IL-14 4.30 PM - 4.50 PM	**Bapu B. Shingate** Assistant Professor, Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, India **Arylidene-Rhodanine/Thiazolidinone Hybrids: Synthesis, Bioevaluation and Molecular Docking Study**
IL-15 4.50 PM - 5.10 PM	**Farukh Arjmand** Department Of Chemistry, Aligarh Muslim University, Aligarh, India **Molecular design, structural features of new RNA targeted antitumor metallodrugs for cancerchemotherapy**
IL-16 5.10 PM - 5.30 PM	**Rajeev Sakhuja** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan, India **Bile acid Hybrids as Anticancer Agents**
IL-17 5.30 PM - 5.50 PM	**Devesh M Sawant** Asst Professor, Pharmacy, Central University of Rajasthan, Bandarsindri, Ajmer, Rajasthan, India **Pd-CatalyzedAzide-Isocyanide Cross Coupling Reaction: Applications in Medicinal Chemistry and Bioimaging**

Poster Session -I

Chairpersons: Dr. Sanjay Kumar, Dr. Bhagwati Saxena and Ms. Anusree Raval

5.50 PM – 7.00 PM	**Poster Session -I (Poster Numbers 1-125)**

7.00 PM – 8.30 PM	**Cultural Programme**
8.30 PM	**Dinner**

Thursday, January 23, 2020

Parallel Session – IVA

Chairpersons: Dr. Surya Prakash Gupta and Dr. Shital Butani

PL-4 9.00 AM - 9.30 AM	**Michele Vittadello** Professor of Chemistry, Medgar Evers College, of the City University of New York, Energy Nanotechnology and Materials Chemistry Team, Brooklyn, NY, USA **Cytochrome *c* Oxidase Oxygen Reduction Reaction induced by Cytochrome *c* on Nickel-Coordination Surfaces based on Graphene Oxide in Suspension**
IL-18 9.30 AM - 9.50 AM	**Ashok K Prasad** Department of Chemistry, University of Delhi, Delhi, India **Sugars to Flavonoids and Other Molecules of Important Applications**
IL-19 9.50 AM - 10.10 AM	**Ashoke Sharon** Associate Professor, Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Computational Studies on HSP90 inhibitors as possible anti-HIV agents**
IL-20 10.10 AM - 10.30 AM	**Amjad Ali** Professor & Head, School of Chemistry and Biochemistry, Thapar Institute of Engineering & Technology, (Deemed to be University), Patiala, India **Transesterification/esterification reactions catalyzed by heterogeneous catalysts to form biofuel and fuel additives**
IL -21 10.30 AM - 10.50 AM	**Debasish Mandal** School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Orientated External Electric Field: An Invisible Catalyst in Bio(Chemical) Reaction**
IL -22 10.50 AM - 11.10 AM	**Luxami, V.** School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, India **Experimental and theoretical investigation of ESIPT based Hydroxy-aryl benzimidazoles/Schiff bases as chromofluorescent sensor**
IL -23 11.10 AM -11.30 AM	**Manik Pradhan** S N Bose National Centre for Basic Sciences, Kolkata, India **Cavity-enhanced absorption spectroscopy in gas and condensed phases: Applications to medical diagnosis**
11.30 AM - 11.40 AM	**High Tea**

Parallel Session – IVB

Chairpersons: Dr. Nandkishor N. Karade and Dr. Bhoomika Patel

PL-5 9.00 AM - 9.30 AM	**Athina Geronikaki** Aristotle University, School of Pharmacy, Thessaloniki, Greece **Dithioloquinolinethiones as new potential multitargeted antibacterial and antifungal agents: synthesis, biological evaluation and molecular docking studies**
IL-24	**Namrata Rastogi**

9.30 AM - 9.50 AM	Scientist, Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Hantzsch Ester Mediated Reactions under Visible Light Irradiation**
IL -25 9.50 AM - 10.10 AM	**Shovan Mandal** Assistant Professor in Chemistry, Syamsundar College, Shyamsundar, Burdwan, India **Palladium-CatalyzedSynthesis of Sulfur Heterocyclesand Their Biological Significance**
IL -26 10.10 AM - 10.30 AM	**Dina Nath Singh** Associate Professor, Department of Chemistry, K.S.Saket PG College, Dr. RML Avadh University, Ayodhya, India **Current Trends Leading to the Isolation of Novel Bioactive Lead Molecules for *Drug Discovery* from *Medicinal Plants***
IL -27 10.30 AM -10.50 AM	**Neelima Gupta** Department of Chemistry, University of Rajasthan, Jaipur, India **Computational Identification of Antiretroviral Drug Candidates through Recognition of HIV(type 1) Conserved Glycoprotein Sequence**
IL -28 10.50 AM -11.10 AM	**Dinesh Kumar Yadav** Assistant Professor, Department of Chemistry, Mohanlal Sukhadia University, Udaipur, India **Graphene Oxide Promoted a Novel Multicomponent Reaction for the Synthesis of 3-Substituted Quinazolinones Using DMSO as One Carbon Source**
IL -29 11.10 AM -11.30 AM	**Asha Jain** Department of Chemistry, University of Rajasthan, Jaipur, India **Synthesis and spectroscopic characterization of some organic-inorganic hybrid complexes of organotin(IV) incorporating the anti-microbial activity analysis**
11.30 AM - 11.40 PM	**High Tea**

Parallel Session-VA

Chairpersons: Dr. Sudhir Kumar Singh and Dr. Jigar Shah

PL-6 11.40 AM - 12.10 PM	**Marco L. Lolli** Assistant Professor in Medicinal Chemistry, Dept. Science and Drug Technology - University of Turin (UniTO), Italy **Effective use of a bioisosteric toll based on hydroxyazolesystems to design inhibitors of *human*Dihydroorotate Dehydrogenase (*h*DHODH) and of other oncological targets**
IL-30 12.10 PM - 12.30 PM	**Virinder S. Parmar** Bioorganic Laboratory, Department of Chemistry, University of Delhi (India); Department of Chemistry and Environmental Science, Medgar Evers College, The City University of New York, USA **Natural products-inspired discovery and development of novel antifungal and antibacterial agents**

IL-31 12.30 PM - 12.50 PM	**Indresh Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **Linear dicarbonyls as suitable substrates for amine catalyzed transformations: Synthesis of medium-sized *N*-heterocyclic compounds**
IL-32 12.50 PM - 1.10 PM	**Deepti Goyal** Department of Chemistry, Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab, India **A multifunctional therapeutic approach: design, synthesis and identification of novel multitarget–directed ligands against Alzheimer's disease**
IL-33 1.10 PM - 1.30 PM	**Satpal Singh Badsara** S Assistant Professor, MFOS Laboratory, Department of Chemistry (Centre of Advanced Study), University of Rajasthan, JLN Marg, Jaipur, Rajasthan, India **Metal-Free Carbon-Sulfur and Phosphorus-Chalcogenides Bond Formations**
1.30 PM - 2.30 PM	**Lunch**

Parallel Session - VB

Chairpersons: Prof. Mahesh Sharma, Dr. Babita Malik and Dr. Dipal Gandhi

IL-34 11.40 AM - 12.00 PM	**Harsha Rajapakse** Department of Chemistry and Environmental Science, Medgar Evers College, The City University of New York, Brooklyn, New York, USA **Time gated Long-lifetime Lanthanide Luminescence to Study Dynamic Molecular Interactions with Improved Resolution**
IL-35 12.00 PM - 12.20 PM	**Dhananjay V Mane** Professor in chemistry and Regional Director, Yashvantrao Chavan Maharastra Open University, Nashik, India **Development and Validation of Analytical Methods for drugs used in treatment of Alzheimer's (Memantine HCl) and Depression Disease (Nortriptyline HCl)**
IL-36 12.20 PM - 12.40 PM	**Hitendra. M. Patel** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar,Gujarat, India **Impact of Green matrix towards the Expansion of Miscellaneous Heterocyclic Scaffolds and their Biological significance**
IL-37 12.40 PM - 1.00 PM	**Ravi P. Singh** Department of Chemistry, Indian Institute of Technology-Delhi, New Delhi, India **Organo and Photoredox Catalysis forC-C bond formation**
IL-38 1.00 PM - 1.20 PM	**Ram Sagar Misra** Associate Professor, Department of Chemistry, Banaras Hindu University, Varanasi, India **Stereoselective Synthesis of Natural Product Inspired New Bioactive Glycohydrids**
IL-39 1.20 PM - 1.40 PM	**Alka Sharma** Centre of Advanced Study, Department of Chemistry, University of Rajasthan,

	Jaipur, India **GREEN NANO MATERIALS FOR SUSTAINABILITY**
1.40 PM - 2.30 PM	**Lunch**

Parallel Session – VIA

Chairpersons: Dr. Rajiv Sharma and Dr. Snehal Patel

PL-7 2.20 PM - 2.50 PM	**Kottawa Gamage Anoja Priyadarshani Attanayake** Head and Senior Lecturer, Department of Biochemistry, Faculty of Medicine, University of Ruhuna, Karapitiya, Galle, Sri Lanka **Nano-encapsulation in herbal nutraceutical applications**
IL-40 2.50 PM - 3.10 PM	**Mandar Bodas** Solution Consultant, Research Solutions - Life Sciences, Elsevier, India **Role of Elsevier Life Science Solutions in Drug Discovery Process**
IL-41 3.10 PM - 3.30 PM	**Arun K. Sinha** Medicinal and Process Chemistry Division, C.S.I.R- Central Drug Research Institute, Lucknow, India **An Innovation Process and Concerns of Green Chemistry: Natural-product-inspired Pot-economy Synthesis of Small Molecules of Biological and Industrial Relevance**
IL-42 3.30 PM - 3.50 PM	**Vikas Tyagi** School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Development of green methodologies in organic synthesis**
O-1 3.50 PM - 4.00 PM	**Nigam M. Mishra** Department of Pharmaceutical Sciences, UNT System College of Pharmacy, University of North Texas Health Science Center, Fort Worth, TX, USA **Asymmetric syntheses identify preferred stereochemistry in small molecule allosteric modulators of the neuropeptide Y4 receptor**
O-2 4.00 PM - 4.10 PM	**Rahul Shivahare** Division of Molecular Parasitology and Immunology and 2Division of Medicinal and Process Chemistry, CSIR-Central Drug Research Institute, Lucknow, India **Strategies for Antileishmanial Drug Development: *De novo* Drug Discovery and Drug Repurposing**
O-3 4.10 PM - 4.20 PM	**Banoth Karan Kumar** Medicinal Chemistry Research Laboratory, Department of Pharmacy, BITS Pilani, Pilani Campus, Pilani, Rajasthan, India ***In-silico* target identification of novel anti-leishmanial β-carboline analogues**
O-4 4.20 PM - 4.30 PM	**Komal M. Vyas** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **Versatile Arene-Ruthenium(II)-Phosphine Complexes: From Green Catalysts for Hydration of Nitriles to Anticancer Agents**

4.30 PM - 4.40 PM	**Tea**

Parallel Session – VIB

Chairpersons: Dr. Anand S. Aswar and Dr. Mohit Shah

IL-43 2.20 PM - 2.40 PM	**Rachna Sadana** Assistant Professor of Biology and Biochemistry, Department of Natural Sciences, University of Houston-Downtown, One Main Street, Houston, TX, USA **Strategies to Engage Undergraduates in Meaningful STEM Research**
IL-44 2.40 PM -3.00 PM	**Bhupesh Goyal** Assistant Professor, School of Chemistry & Biochemistry, Thapar Institute of Engineering & Technology (Deemed to be University), Patiala, Punjab, India **Computational screeningof potential inhibitors against β_2m aggregation in Dialysis-related amyloidosis**
IL-45 3.00 PM - 3.20 PM	**Ramendra Pratap** Department of Chemistry, University of Delhi, North campus, New Delhi, India **Synthesis of various carbocycles and heterocycles from functionalized benzyl cyanide**
IL-46 3.20 PM - 3.40 PM	**Devdutt Chaturvedi** Head, Department of Chemistry, School of Physical Sciences, Mahatma Gandhi Central University (MGCU), Motihari, Distt.: East Champaran, BIHAR, India **Carbon disulfide: Greener syntheses for biologically potent scaffolds**
O-5 3.40 PM - 3.50 PM	**Molisha Soni** Department of Pharmacology, Institute of pharmacy Nirma University, Ahmedabad, India **EVALUATION OF *EUPHORIA LONGANA* IN ORAL CANCER INDUCED RATS ASSOCIATED WITH TYPE II DIABETES MELLITUS**
O-6 3.50 PM - 4.00 PM	**Malek Mohammed Abrar Hafijmiya** Department of Industrial Chemistry, VP & RPTP Science College. Vallabh Vidyanagar, Anand, Gujarat, India **DIVERSE STRATEGIES TO BOOST UP SOLUBILITY OF POOR WATER SOLUBLE DRUGS - A REVIEW**
O-7 4.00 PM - 4.10 PM	**Pratibha Yadav** Centre for Rural Development and Technology, IIT Delhi, Hauz Khas, New Delhi, India **Transformation of Different Sulfides to its Sulfoxide by a Plant Peroxidase**
O-8 4.10 PM - 4.20 PM	**Kamna Goel** School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India **Synthesis and *in vitro* pharmacological characterization of pyrimidinium ionic liquids**

O-9 4.20 PM - 4.30 PM	**Balaram S. Takale** Department of Pharmaceutical Sciences and Technology, Institute of Chemical Technology, Mumbai, India **Highly sustainable approach towards synthesis of pharmaceutically relevant molecules**
4.30 PM - 4.40 PM	**Tea**

Parallel Session – VII A

Chairpersons: Prof. Man Singh and Dr. Dhaivat Parikh

PL-8 4.40 PM - 5.10 PM	**Laurent El Kaim** Laboratoire de Synthèse Organique, Ecole Polytechnique, Palaiseau, France **Post-condensations of Ugi adducts: a step towards higher diversity**
IL-47 5.10 PM - 5.30 PM	**Sunil Jambhekar** Professor of Pharmaceutical Sciences, LECOM School of Pharmacy, 5000 Lakewood Ranch Boulevard Bradenton, Florida, USA **Abstract Awaited**
IL-48 5.30 PM - 5.50 PM	**Surendra Singh** Assistant Professor, Dept. of Chemistry, University of Delhi, Delhi, India **Development of Chiral catalysts for Asymmetric Organic Reactions**
O-10 5.50 PM - 6.00 PM	**Prem Kumar Kushwaha** Department of Chemistry, Birla Institute of Technology Mesra, Ranchi, India **Synthesis of Therapeutic significant oxadiazole analogs and its crystallographic studies**
O-11 6.00 PM - 6.10 PM	**Nisha Kumari** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Studies on Moringa based flocculant for the treatment of wastewater**
O-12 6.10 PM - 6.20 PM	**Rajat Kumar Pandey** Department of Pharmaceutics,Schoolof Pharmaceutical Sciences, Shoolini University, Solan, HP, India **Synthesized and computational prediction of furfuraldehyde-sulfonamide Schiff base compounds and their antibacterial activity**

Parallel Session – VII B

Chairpersons: Prof. Hitesh D. Patel and Dr. Bhumika Patel

IL-49 4.40 PM - 5.00 PM	**Sartaj Tabassum** Department of Chemistry, Aligarh Muslim University, Aligarh, India **New Metal Based Pharmaceuticals, Structural Characterisation and their Anti-cancer activity**
IL-50 5.00 PM - 5.20 PM	**Prakash C. Jha** Associate Professor & Chairperson, Centre for Applied Chemistry, Central University of Gujarat, Gandhinagar, India

	Druggable Space beyond the rule of 5
IL-51 5.20 PM - 5.40 PM	**Nighat Fahmi** Department of Chemistry, University of Rajasthan, Jaipur, Rajasthan, India **Evaluation of Antimicrobial, DNA cleavage and anticancer activities of transition metal Schiff base complexes**
O-13 5.40 PM - 5.50 PM	**Raj Kumar Das** School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, India **Metal-Organic Frameworks as New General Catalyst for Electrochemical Water Splitting**
O-14 5.50 PM - 6.00 PM	**Lata Rani** Department of Chemistry, Indian Institute of Technology Gandhinagar, Gandhinagar, Gujarat, India **Conformational influences of Phosphorylation and O-GlcNAcylation on Proline-rich domain of Tau**
O-15 6.00 PM - 6.10 PM	**Riya Sailani** Department of Chemistry, University of Rajasthan, Jaipur, India **ENTHALPY-ENTROPY COMPENSATION (EEC) EFFECT IN REDOX KINETICS BETWEEN PARA-SUBSTITUTED ANILINE AND PEROXOMONOSULFATE IN ACIDIC MEDIUM**

Poster Session -II

Chairpersons: Dr. Brijesh Kumar Srivastava, Dr. Jawahar Lal and Dr. Pradeep Srivastava

6.20 PM – 8.00 PM	**Poster Session -II (Poster Numbers 125 onwards)**
8.00 PM	**Dinner**

Friday, January 24, 2020

Parallel Session –VIIIA

Chairpersons: Prof. Diwan Singh and Dr. Charmy Kothari

PL-9 9.00 AM – 9.30 AM	**Vassilios Papadopoulos** Dean, School of Pharmacy, John Stauffer Dean's Chair in Pharmaceutical Sciences. Professor of Pharmacology & Pharmaceutical Sciences, University of Southern California, Los Angeles, California, USA **Understanding the biology and designing new therapeutic approaches for the treatment of male hypogonadism**
IL-52 9.30 AM - 9.50 AM	**Ravindra Kumar** Scientist, CSIR-Central Drug Research Institute, Lucknow, India **Catalytic and Enantioselective Synthesis of Benzoxasiloles: Direct Application to (*R*)-Orphenadrine and (*S*)-Neobenodine**

IL-53 9.50 AM - 10.10 AM	**Asit K. Chakraborti** Professor and Head, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), S. A. S. Nagar, Punjab, India **Integrating Sustainable Chemistryin Pharmaceutical Research: Novel Transition Metal-free Approaches for Drug Discovery and Development**
IL-54 10.10 AM -10.20 AM	**Tejal Mehta** Dept. of Pharmaceutics, Institute of Pharmacy, Nirma University, Ahmedabad, India **Nanocrystal Based Topical Formulations for the Treatment of Fungal Infections**
O-16 10.20 AM -10.30 AM	**Vikki N. Shinde** Department of Chemistry, BITS Pilani, Pilani Campus, Pilani, Rajasthan, India **Design and Syntheses of Palladium Complexes of NNN/CNN Pincer Ligands for Catalytic Dehydrogenative Cross-Coupling of Heteroarenes**
O-17 10.30 AM -10.40 AM	**Pidiyara Karishma** Department of Chemistry, Birla Institute of Technology & Science, Pilani, Rajasthan, India **Ruthenium Catalyzed C-H Acylmethylation of *N*-Arylphthalazine-1,4-diones with *α*-Carbonyl SulfoxoniumYlides: Highway to Diversely functionalized Phthalazino-fused Cinnolines**
O-18 10.40 AM -10.50 AM	**Saroj Yadav** Department of Chemistry, University of Delhi, North Campus, Delhi, India **Agreen synthesis of multifunctional thieno(3,2-*c*)pyran-4-ones from 2-pyranones**
O-19 10.50 AM -11.00 AM	**Bhumika D. Patel** Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India **3D-QSAR and Ligand Based Pharmacophore Modelling of Poly ADP-Ribose Polymerase 1 (PARP1) Inhibitors**
11.00 AM - 11.20 AM	**High Tea**

Parallel Session –VIII B

Chairpersons: Prof. Dalip Kumar and Ms. Palak Parikh

IL-55 9.00 AM – 9.20 AM	**Sanjib Bhattacharyya** Department of Pharmaceutical Science and Chinese Traditional Medicine, Southwest University, 2 Tiansheng Rd, Beibei Qu, Chongqing Shi, China **Meeting the neurodegenerative disease at the junction of chemical, biological and behavioral science**
IL-56 9.20 AM - 9.40 AM	**T. Narender** Principal Scientist, Medicinal and Process Chemistry Division , CSIR-Central Drug Research Institute, Lucknow, India **CHEMICAL AND BIOLOGICAL EXPLORATION OF INDIAN MEDICINAL PLANTSFOR HUMAN HEALTH CARE**

IL-57 9.40 AM - 10.00 AM	**Sushil Kumar Maurya** Natural Product Chemistry and Process Development Division, CSIR-Institute of Himalayan Bioresource Technology, Palampur, Himachal Pradesh, India **DIVERSITY ORIENTED SYNTHESIS APPROACH FOR MACROCYCLES**
IL-58 10.00 AM - 10.20 AM	**Rodney A. Fernandes** Professor, Chemistry Department, IIT Bombay, Powai Mumbai, India **Unique Rearrangements of β-Aryloxyacrylates and δ-Hydroxy-alkynones Under Mild Acid Catalysis**
IL-59 10.20 AM - 10.30 AM	**Niyati Acharya** Dept. of Pharmacognosy, Institute of Pharmacy, Nirma University, Ahmedabad, India **Beneficial effects of Bergenin in Alzheimer's disease: In silico, in vitro and invivo evaluation**
O-20 10.30 AM - 10.40 AM	**Areeg Anwer Ali** Departmentof Clinical Pharmacy and Pharmacology, Rak College of Pharmaceutical Sciences, RAK Medical and Health Sciences University, Ras Al Khaimah, United Arab Emirates **Assessment of Implementation of Antibiotic Stewardship Program in Surgical Prophylaxis at a Secondary Care Hospital in Ras Al Khaimah, United Arab Emirates**
O-21 10.40 AM - 10.50 AM	**Ankita Rai** School of Physical Sciences, Jawaharlal Nehru University, New Delhi, India **FACILE Cu (I)-INDUCED ACTIVATION OF FURAN TO [4+2] AZA-DIELS-ALDER REACTION FOR SYNTHESIS OF TETRAHYDROPYRIDINES**
O-22 10.50 AM - 11.00 AM	**Bintu Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **RegioselectiveSynthesis and PhotophysicalStudies of Triazolyl Boron-dipyrromethene Complexes**
11.00 AM - 11.20 AM	**High Tea**

Parallel Session –IX A

Chairpersons: Dr. Ravindra V. Singh and Dr. Mayur Patel

IL-60 11.20 AM –11.40 AM	**Saranjit Singh** Dean Professor & Head, Pharmaceutical Analysis, National Institute of Pharm. Education & Research, NIPER, S.A.S. Nagar (Mohali), India **Model Informed Precision Dosing for Pediatric Population**
IL-61 11.40 AM - 11.50 AM	**Priti Mehta** Dept. of Pharmaceutical Analysis, Institute of Pharmacy, Nirma University, Ahmedabad, India **Human space medicine: stability issues with case studies and countermeasures**

O-23 11.50 PM - 12.00 PM	**Pratibha Singh** MFOS Laboratory, Department of Chemistry (Centre of Advanced Study), University of Rajasthan, Jaipur, Rajasthan, India **Substrate-switched dual functionalization of alkenes: catalyst-free synthetic route for *β*-hydroxy and *β*-ketothioethers**
O-24 12.00 PM - 12.10 PM	**Jobin Jose** Department of Pharmaceutics, NITTE Gulabi Shetty Memorial Institute of Pharmaceutical Sciences, NITTE Deemed-to-be University, Mangalore, India **DEVELOPMENT, CHARACTERIZATION AND EVALUATION OF SOLID LIPID NANO PARTICLES OF *ALOE VERA***
O-25 12.10 PM - 12.20 PM	**Amol Prakash Pawar** Department of Chemistry, BITS, Pilani, Rajasthan, India **Enantio- and Diastereoselective Two-Pot Synthesis ofIsoquinuclidines from Glutaraldehyde and N-Aryl Imines with DFT-Calculations**
O-26 12.20 PM - 12.30 PM	**Anu Manhas** School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India **A novel attempt to explore the pharmacophoric space of the enzymatic proteome of *Plasmodium falciparum* using multicomplex-based pharmacophore modeling**
O-27 12.30 PM - 12.40 PM	**Chandralata Bal** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Synthesis of Entecavir-Aristeromycin Hybrid Scaffold as anti-HBV Agents**
O-28 12.40 PM - 12.50 PM	**Rekha Bai** MFOS Laboratory, Department of Chemistry (Centre of Advanced Study), University of Rajasthan, Jaipur, Rajasthan, India **Highly Atom-Economic, Catalyst-free, and Solvent-free Phosphorylation of Chalcogenides**
O-29 12.50 PM - 1.00 PM	**Mohd Jubair Aalam** Department of Chemistry, University of Delhi, Delhi, India **Development of Modified MacMillan based Ionic liquids as organocatalystfor Asymmetric Friedel-Crafts Reaction**

Parallel Session –IX B

Chairpersons: Prof. Athina Geronikaki and Dr. Nrupesh Patel

IL-62 11.20 AM - 11.40 AM	**Siddharth Sharma** Assistant Professor, Department of Chemistry, Mohanlal Sukhadia University, Udaipur, India **Isocyanide Insertion Reactions: Our Findings**
IL-63 11.40 AM - 11.50 AM	**Jigna Shah** Dept. of Pharmacology, Institute of Pharmacy, Nirma University, Ahmedabad, India **Involvement of PTEN expression in antitumour activity of febuxostat against 4-Nitro quinolone induced oral cancer in rats**

O-30 11.50 AM - 12.00 PM	**Faraz Shaikh** Department of Computer and Information Science, University of Macau **LigTMap: Ligand and Structure-Based Target Identification and Activity Prediction for Small Molecules**
O-31 12.00 PM - 12.10 PM	**Dinesh Kumar** School of Chemical Sciences, Central University of Gujarat, Gandhinagar, India **Visual Detection of Aqueous Health Hazard Ions**
O-32 12.10 PM - 12.20 PM	**Jignesh P. Raval** The Mandvi Education Society Science College (TMES), Mandvi, Gujarat, India **Ultrasound promoted synthesis of Novel benzothiazinone derivatives and its pharmacological evolution**
O-33 12.20 PM - 12.30 PM	**Ravi Pal** Center for DNA fingerprinting and diagnostics, Hyderabad, Telangana, India **PPE2: a blessing in disguise**
O-34 12.30 PM - 12.40 PM	**Anurag Zaveri** Department of Biotechnology, KadiSarvaVishwaVidyalaya, Gandhinagar, India **Isolation, screening and molecular characterization of multidrug resistant organisms, to screen and identify carbapenem producers, from operation theaters and Intensive Care Unitsof Ahmedabad**
O-35 12.40 PM - 12.50 PM	**Ruby Kharwar** Ashok and Rita Patel Institute of Integrated Study and Research in Biotechnology and Allied Sciences (ARIBAS), New Vallabh Vidyanagar, India **8-HYDROXYQUINOLINE-SULFONAMID HYBRIDE LIGAND AND ITS METAL CHELATES: SYNTHESIS, CHARACTERIZATION, *IN SILICO* ADMET, *IN VITRO* ANTIMICROBIAL, DNA INTERACTION AND MOLECULAR DOCKING STUDIES**
O-36 12.50 PM - 1.00 PM	**Vishnu Prabhakar Srivastava** National Sugar Institute, Kanpur, Uttar Pradesh, India **Direct Use of Sugarcane bagasse derived hemicellulose hydrolysate for the synthesis of *C*-glycosyl derivatives by the Lubineau Reaction**
O-37 1.00 PM - 1.10 PM	**Khandhara Vraj** M.Pharm in Regulatory Affairs, Department of Pharmaceutical Analysis Institute of Pharmacy, Nirma University, Ahmedabad, India **REGULATORY COMPLIANCE MANAGEMENT OF TRANSDERMAL PATCHES**

1.10 PM - 2.00 PM	**Valedictory Session**
2.00 PM –3.00 PM	**Lunch**

- End of Programme -

PLENARY

PL-1

Building Better Enzymes: Redesigning DNA Polymerases to Replicate Nucleobases in Expanded Genetic Alphabets

Nigel Richards

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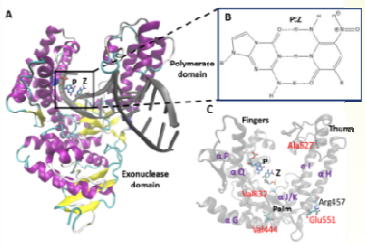
Abstract: The development of "semi-synthetic" microorganisms possessing artificially expanded genetic information systems (AEGIS) will permit access to cells with novel phenotypes and biotechnological applications [1]. Non-natural nucleobase pairs that meet the size and/or hydrogen bonding complementarity rules of Watson-Crick base pairing include the complementary 2-amino-8-(1-beta-D-2′-deoxyribofuranosyl)imidazo [1,2-a]-1,3,5-triazin-[8H]-4-one (trivially known as **P**) and 6-amino-3-(2′-deoxyribofuranosyl)-5-nitro-1H-pyridin-2-one (trivially known as **Z**) nucleobase pair that is present in "hachimoji" DNA (Figure). As is true of naturally occurring (Watson-Crick) DNA, AEGIS DNA duplexes containing **P**:**Z** pairs interconvert easily between A- and B-helical forms [2,3]. In addition, B-form DNA tolerates the inclusion of multiple consecutive **P**:**Z** nucleobase pairs with minimal structural impact on the double helix when compared to duplexes containing only A:T or G:C base pairs [4]. The high-resolution X-ray crystal structure of a KlenTaq variant has been reported [5] that incorporates the "hachimoji" **P**:**Z** nucleobase pair with a similar efficiency to that seen for Watson-Crick nucleobase incorporation by wild type (WT) KlenTaq DNA polymerase. The variant polymerase differs from WT KlenTaq by only four amino acid substitutions, none of which are located within the active site (Figure).



*(A) Cartoon representation of the X-ray crystal structure of the variant KlenTaq polymerase in its binary complex (PDB: 5W6Q) [5] showing the location of **P**:**Z** in the active site. (B) The **P**:**Z** nucleobase pair. (C) Close-up of the polymerase domain showing the side chains of mutated residues, Val444, Ala527, Glu551 and Val832, in the Klentaq variant.*

This lecture will present new research aimed at extending the number of nucleobase pairs that can be used to encode proteins together with insights into how the presence of AEGIS nucleobases affects the structural properties of duplex DNA. I will also discuss structural and computational studies that elucidate the contributions of the four amino acid substitutions to the altered catalytic activity of the polymerase [6]. Computational methods have a clear role to play in systematically screening DNA polymerase variants capable of incorporating non-natural nucleobases thereby limiting the number that must be characterized by experiment.

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PL-2

BATCH AND CONTINUOUS FLOW CONVERSION OF BIOMASS INTO FURAN DERIVATIVES

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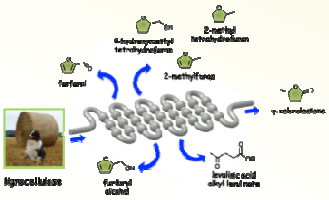
Abstract: The concepts of sustainable development, bio-economy and circular economy are increasingly being applied to the synthesis of molecules of industrial interest. Among these molecules, furfural as a platform molecule is the subject of various research approaches to improve its synthesis and productivity, and also to extend its transformation for the production of molecules of interest. Due to the current momentum in promoting green chemistry for sustainable development, chemists have recently established catalytic reactions based on alternative technologies such as continuous flow.

The present study showed recent breakthroughs obtained in the production of furfural [1-10], hydroxymethylfuran [11-13], methylfuran [11-13], methyl levulinate [14] and -valerolactone [15] starting from lignocellulose in the presence of homogeneous catalysts and heterogeneous catalysts using either batch process or continuous flow process. Various reaction parameters in dependence of time such as temperature, catalyst and feedstock loadings as well as solvent types have been optimized.

Conception, synthesis and physico-chemical properties will be detailed.



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PL-3

New Strategies for Design and Development of Neutral and Hydrophobic Extrinsic Fluorescent Probes

Anil K Singh

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Abstract: *Fluorescent probes (FPs) are molecular entities, extensively used for studying the microenvironments by applying different techniques of fluorescence spectroscopy [1,2]. Among their myriad of uses, FPs are used in probing structure, biomolecular binding and interactions, cellular imaging,biological events and dynamics, and discover new drugs, etc. to name but a few. FPs can be broadly grouped in two categories: i) intrinsic FPs, which are primarily based on biomolecules like the amino acids, proteins, antibodies, etc., and ii) extrinsic FPs, which are based on synthetic small organic molecules, select proteins, quantum dots, etc. In general, a good fluorescent probe (FP) is characterized by its maximum λ_{abs} and λ_{em} wavelength, high extinction coefficient, high fluorescence Φ_f, proper interaction with the host system, large Stokes' shift, ability to undergo change in its fluorescence behavior in response to change in its surroundings, etc. Both, intrinsic as well as extrinsic, FPs suffer from a few disadvantages. For instance, in the case of intrinsic FPs the disadvantage could be due to probe's inadequate fluorescence efficiency, wavelength range, sensitivity, ability to provide proper information in the presence of multiple fluorophores in the system. Similarly, in the case of a biological extrinsic FP the problem could arise due to probe's generally large molecular size, artifactual response, photoinstability. To alleviate some of the problems, small organic molecules bearing appropriate fluorophore have been considered for use as extrinsic FP. These probes are based on several structural frameworks such as naphthyl, fluorescein, pyrenes, anthraquinones, triarylmethane derivatives, oxadiazoles, cyanine derivatives, benzoxathioles, tetrapyrrole derivatives, acridine derivatives, xanthenes, coumarins, etc. However, several of these probes also suffer from shorter λ_{abs} and λ_{em} wavelength, and some of these are charged, hydrophilic and have self-ionic behaviour, which limits their biological and medical applications. The fluorescence information obtained from the charged FPs may be due to ionic/ secondary Columbic interactionsthat these probes undergo with the host, and this interferes with the fluorescence studies and complicates fluorescence data interpretation.*

Considering the aforesaid, attempts have been made towards designing neutral and hydrophobic extrinsic FPs based on small synthetic organic molecules. In one such attempts, **the efficacy of α,ω-diarylpolyenes as neutral, hydrophobic extrinsic FP has been explored [3]. It is based on the fact that dipolar excited states are involved in the photoprocesses of linear polynes [4]. Thus, fluorescence behaviour of a number of** diaryl ethenes, **diarylbutadienes and styryl indoles have been examined. It has been found that these compounds are capable of exhibiting efficient solvent polarity- and substituent-dependent fluorescence, despite the fact that ethenes and linear polyenes in general do not fluoresce due to availability of alternate channel for excited state energy dissipation, *e.g.*through C=C isomerization. It has been further observed that i**n general compounds bearing donor or acceptor groups fluoresce from their locally excited state, and those substituted with both strong donor and acceptor groups show solvent polarity- and substituent-dependent dual fluorescence from their **conformationally relaxed intramolecular charge transfer excited state (Fig.1). Interestingly, the** styrylindoles also exhibit aggregation-induced enhanced fluorescence in the **solid state** due to specific molecular arrangement in the crystal. These compounds also show dramatically enhanced fluorescence in the nanoparticle forms. **The efficacy of these compounds as neutral, hydrophobic FPs is amply demonstrated by FP studies of proteins and micelles.Attempts are also underway to design** two-photon excitable (TPE) chromophores, which owing to lower energy of employed photons, cause less photo-damage and photo-bleaching to the biological systems than the corresponding one-photon microscopy. TPE compounds have brought

new dimensions to fluorescence probing, wherein lies a great scope for design and development of TPE probes for biological applications.

This talk, while presenting a detailed discussion of the aforesaid aspects of FPs, would accentuate on the importance of detail mechanistic knowledge of the excited state in FP design and would uncover design and development of **neutral, hydrophobic extrinsic fluorescent probes based on** excited state stereo-electronic considerations of **synthetic α,ω-diarylpolyenes.**

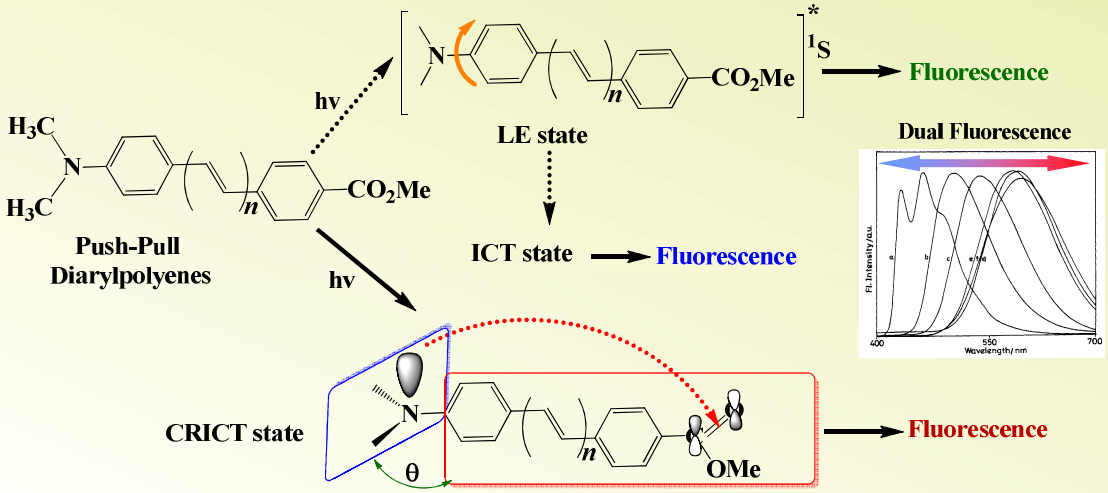

Fig. 1. LE, ICT and CRICT fluorescent excited states of α,ω-diarylpolyenes.

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PL-4

Cytochrome *c* Oxidase Oxygen Reduction Reaction induced by Cytochrome *c* on Nickel-Coordination Surfaces based on Graphene Oxide in Suspension

Xiaoping Zhu[a], Erika Aoyama[b], Alexander V. Birk[a,c], OladapoOnasanya[a], William H. Carr[d], Lev Mourokh[e,f], Shelley D. Minteer[b], and Michele Vittadello[a,g,*]

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Abstract: *In vitro* investigations on isolated components of the mitochondrial electron transport chain are expected to shed new light on the plethora of bioenergetic functions carried out by mitochondria, affecting the performance of living organisms. This study is focused on assessing the biocompatibility of graphene oxide (GO) derivatives with His-tagged cytochrome c oxidase (CcO), expressed and purified from *Rhodobactersphaeroides* using the Gibson assembly method. As prepared GO was enriched with carboxylic acid groups yielding carboxylated GO (CGO). CGO was functionalized with nitrilotriacetic acid (NTA) yielding CGO-NiNTA, in the presence of Ni^{2+} ions. We investigated the reaction of horse-heart cytochrome c (Cyt c) with free CcO and CGO-NiNTA-CcO coordination complexes in suspension. Kinetic studies by UV-Visible absorption spectroscopy confirmed that free CcO oxidizes Cyt c and provided a similar indication for immobilized CcO. However, oxygen-consumption measurements using a Clark-type electrode suggested that CGO-based supports are capable of oxygen reduction reaction (ORR), especially in the presence of Ni^{2+} coordination centers. The ORR caused by immobilized CcOcould be clearly distinguished from that of CGO-NiNTA in the presence of Cyt c and dithiothreitol (DTT) as a sacrificial reducing agent. The results indicate that while the protein content is about 3.7 ‰ by mass with respect to the support, the contribution to the oxygen consumption activity ranges from 39.3% to 71.0%, depending on the concentration of DTT. This finding indicates that the support stabilizes the free enzyme which, while capable of Cyt c oxidation, is unable to carry out oxygen consumption in solution under our conditions. The turnover rate was as high as $250O_2$ molecules per second per CcO unit.

PL-5

Dithioloquinolinethiones as new potential multitargeted antibacterial and antifungal agents: synthesis, biological evaluation and molecular docking studies

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Abstract: Herein we report the design, synthesis, molecular docking study and evaluation of antimicrobial activity of ten new dithioloquinolinethiones. The structures of compounds were confirmed by ^{1}H-NMR, ^{13}C-NMR and HPLC-HRMS. Before evaluation of their possible antimicrobial activity prediction of toxicity was performed. All compounds showed antibacterial activity against eight Gram positive and Gram negative bacterial species. All compounds appeared to be more active than ampicillin and almost all than streptomycin. The best antibacterial activity was observed for compound **8c** 4,4,8-trimethyl-5-{[(4-phenyl-5-thioxo-4,5-dihydro-1,3,4-thiadiazol-2-yl)thio]acetyl}-4,5-dihydro-1H-[1,2]dithiolo[3,4c]quino lone-1-thione). The most sensitive bacterium *En.cloacae* followed by *S. aureus*, while *L.monocytogenes* was the most resistant. All compounds were tested for antifungal activity also against eight fungal species. The best activity was expressed by compound **8d** (5-[(4,5-Dihydro-1,3-thiazol-2-ylthio)acetyl]-4,4-dimethyl-4,5-dihydro-1H-[1,2]dithiolo[3,4-c]quinoline-1-thione). The most sensitive fungal was *T. viride*, while *P. verrucosum var. cyclopium* was the most resistant one. All compounds were more potent as antifungal agent than reference compound bifonazole and ketoconazole. The docking studies indicated a probable involvement of *E. coli* DNA GyrB inhibition in the anti-bacterial mechanism, while CYP51ca inhibition is probably responsible for antifungal activity of tested compounds. It is interesting to mention that docking results coincides with experimental.

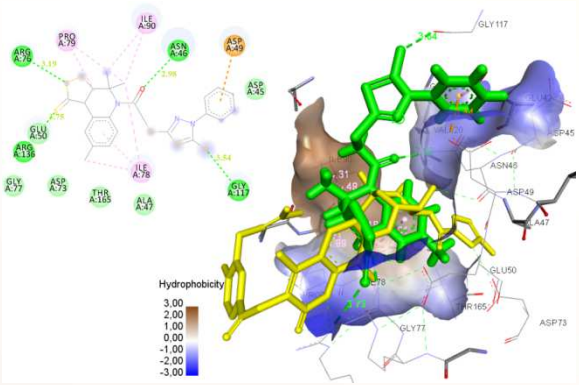

Figure. Docked conformation of the most active compound **8c** (green) and Clorobiocin (yellow) in *E. coli* DNA GyrB.

PL-6

Effective use of a bioisosteric toll based on hydroxyazole systems to design inhibitors of *human* Dihydroorotate Dehydrogenase (*h*DHODH) and of other oncological targets

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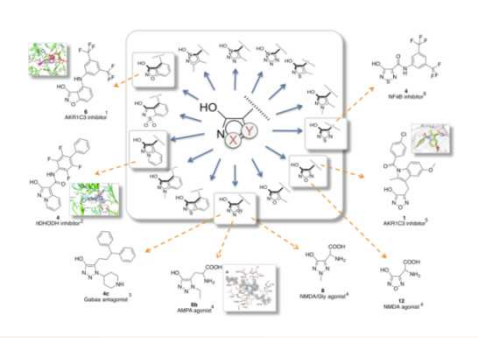
Abstract: During the design of drug candidates, *bioisosterism* is often the winning approach to improve potency/selectivity, achieve optimal ADME-T profiles and acquire novel intellectual property (IP). In some ways, the eternal confrontation between the concepts of *isostere* (defined by a chemistry-related context) and *bioisostere* (defined by a biological-related context) is well representative of the deep soul of a *Medicinal Chemist*. The frequent absence of correlation of biological activity between isosteres is often a brutal remind of how the translation of a chemistry-based design into a living organism context could be challenging.

In the last fifty years, acidic ***hydroxyazoles***, because of their isosteric connection to the carboxylic group, represent an efficient tool for designing active compounds with added IP value. Recently, we and other groups, while expanding the chemical space of these hydroxylated heterocycles, systematically explored these systems in the framework of *hit-to-lead* optimization processes. This contribute, while covering the acidic hydroxyazoles research field and detailsome of their most recent application in *Medicinal Chemistry* (see figure), will be major focused on the design of human dihydroorotate dehydrogenase (*h*DHODH) inhibitors. Being already validated as therapeutic target for the treatment of autoimmune diseases, in the fall 2016 *h*DHODH was associated to *acute myelogenous leukemia*(AML), a disease that has not seen a new therapies in four decades.This discovery opened a totally new prospective in *h*DHODH and AML field. Starting from *brequinar*, one of the most potent known *h*DHODH inhibitors, and by applying innovative *scaffold-hopping* replacement, we recently designed a novel generation of potent and selective *h*DHODH inhibitors presentingnano-molar activity on theisolated *h*DHODH able to restore the myeloid differentiation in leukemia cell lines, in a range superior then brequinar itself. Theoretical design, modeling, synthesis, SAR, X-ray crystallographic poses, biological assays (cell viability, proliferation, cytotoxicity, immunosuppression, myeloid differentiation), ADME and *in vivo* toxicity and efficacy are here presented and discussed.



References:

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PL-7

Nano-encapsulation in herbal nutraceutical applications

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Abstract: Nutraceuticals are molecules which shade the frontier between drugs and food. Molecules used in nutraceuticals possess interesting and often potent biological activities but also can be scaffolds for synthetic derivatives, significantly reducing the time and cost of development of new molecules with therapeutic potential. Nutrients, herbals and dietary supplements are major constituents of plant based nutraceuticals which make them instrumental in maintaining health, act against various diseases and thus promote the quality of life.

Nano-encapsulation is an innovative approach that has potential applications in nutraceutical research. Nanoparticles have proved as one of the logical and encouraging tools for the rapid delivery of drugs/neutraceutcials in controlled and targeted manner. The nanoparticles have the potential to increase solubility due to a combination of a greater surface area and large interfacial adsorption of the core compound. Other benefits of the utilization of nanoparticles include enhanced bioavailability, improved controlled release and better precision targeting of the encapsulated materials. Accordingly, encapsulated food compounds /formulations enhance pharmacokinetic properties, bioavailability and drug targeting in different pathological conditions *in vivo*. Phyto-derived bioactive compounds have been loaded into nanoparticles for oral delivery in various animal models of chronic diseases, and the results have shown improved stability, bioavailability and sustained bioactivities.Recently, research work has been increasingly focused on designing formulations consisting of nanoparticles constituted from different polymers and containing encapsulated plant extracts in order to combine the diversity of bioactivities of plant extracts and the advantages offered by the nanoparticles. Indeed, the use of nanoparticle based formulations to improve biopharmaceutical and chemical properties of plant based nutraceuticals is of current interest worldwide. Delivery systems for hydrophilic bioactive materials or plant extracts include several generally recognized as safe (GRAS) approved materials like lipids, polymers, carbohydrates, proteins that can be used to fabricate nano/micro carrier; however, only a few of them are recommended for regular consumption.In comparison with conventional formulations, nano-formulations can increase the solubility of constituents, reduce the therapeutic dose, and improve absorption of the active components. Nano-nutraceutical formulations targeting the management of chronic diseases would essentially exert particular bioactivities with enhanced targeted delivery to the sites of interest. The potential applications and beneficial effects of nano-encapsulation in herbal nutraceutical formulations in present and future scenarios will be discussed.

PL-8

Post-condensations of Ugi adducts: a step towards higher diversity

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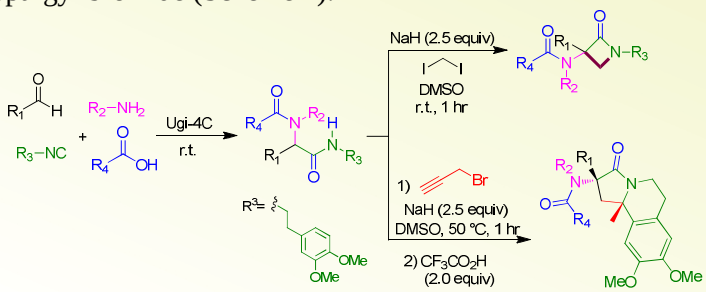
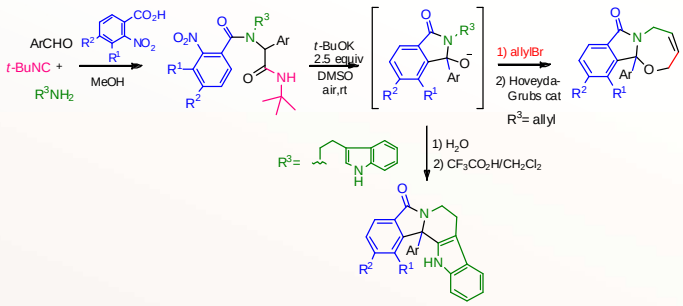
Abstract: Ugi and Passerini Post-condensations are modifications of Ugi and Passerini adducts that traditionally involve intramolecular reactions leading to more or less complex heterocyclic scaffolds. We have been interested in the last few years by performing intra and intermolecular reactions playing on the peptidyl positions of Ugi adducts. While intramolecular reaction at this position are well documented, intermolecular reactions are much more difficult for steric reasons. The formation of amide dianions of Ugi adducts has allowed us to achieve easy room temperature alkylations which have been extended to the disclosure of cascades using bielectrophilic derivatives such as diiodomethane or propargyl bromide (Scheme 1).[1]



Scheme 1

In diversity oriented approach towards heterocycles, the amide moiety coming from the isocyanide is often not considered as the most valuable part as the number of commercially available isocyanides is relatively limited. It is thus interesting to extent the scope of Ugi reactions through transformation of the isocyanide moiety. Working on intramolecular reactions at the peptidyl position, we have proposed an approach involving a fragmentation of the Ugi adduct with removal of the amide as an isocyanate. The resulting loss of diversity may be compensated by a further functionnalisation (Scheme 2).[2]



Scheme 2

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PL-9

Understanding the biology and designing new therapeutic approaches for the treatment of male hypogonadism

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Abstract: Testosterone (T), synthesized by testicular Leydig cells (LCs), is critical for male developmental and reproductive functions, and contributes significantly to quality-of-life and well-being. Reduced serum T is common in aging men, and also occurs in men diagnosed with idiopathic infertility, orchitis, genital trauma, spinal cord injury and testicular torsion, and after chemotherapy or irradiation. Reduced T is associated with mood changes, fatigue, depression, decreased lean body mass, reduced bone mineral density, increased visceral fat, metabolic syndrome, cardiovascular disease, decreased libido, and erectile dysfunction. T replacement therapy (TRT) is used clinically to restore T levels. However, there are alarming reports of possible side-effects associated with TRT, making it desirable to develop additional strategies for increasing T. Unfortunately, there are major gaps in our knowledge of the mechanisms involved in T production and in the changes leading to hypogonadism, making it difficult to develop drugs that might positively affect T synthesis. In this presentation Dr. Papadopoulos will present an overview of recent advances in understanding the mechanisms underlying T biosynthesis in normal and hypogonadal testis that paved the way for the identification of molecular targets and the development of novel pharmacological and stem cell strategies to increase serum T levels by restoring T production in LCs.

INVITED

IL-1

A Dietary Supplement use as An Anti-Aging Agent

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Abstract: Ambitions and attempts to control aging have been part of human culture since early civilizations. The last decay has seen a major transformation in the Anti-aging innovation in cosmetics and pharmaceutical industry. Creating an industry estimated to have an approximate value of $ 39 billion. There are more than 50,000 dietary supplements are marketed. Indeed it opens an opportunity to explore the possibilities of an anti-aging from our dietary supplements. Various dietary supplements / food ingredients are designed for lower cost and eco-friendly manufacturing to meet the global demand. The global anti-aging products market is increased by ~ 7 % against the previous year. Anti-aging research is reflecting scientific talent in its application and the large-scale manufacturing.

IL-2

CYCLO OLEFIN POLYMER, THE NEW AGE MATERIAL FOR MEDICAL APPLICATION BY ZEON: OUTLINE OF ZEON MEDICAL PRODUCT

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Email: S.Chauhan@zeon.co.jp.

Abstract: Cyclo olefin polymer (COP) is a high performance thermoplastic that overcomes limitations of traditional packaging materials.The COP material of ZEON has commercialized by trade names ZEONEX® and ZEONOR® (1, 2). ZEONEX® and ZEONOR® are mainly prepared by ring opening metathesis polymerization (ROMP) of cyclo olefin followed by hydrogenation.

ZEONEX® medical product is promising that they have very pure, amorphous, low protein adsorption, and high transparent and nonpolar plastic with excellent chemical resistance and moisture barrier. ZEONEX®popularly used as medical vials, syringes, syringes pre-filled with pharmaceutical content, and packaging that also serves to protect tablet pharmaceuticals. In the figure 1(a) shows ZEONEX® prefilled syringe have low protein adsorption than glass medical product. Figure 1(b) prefilled syringe picture made by ZEONEX®. We will discuss detail of ZEONEX® medical products during conference.

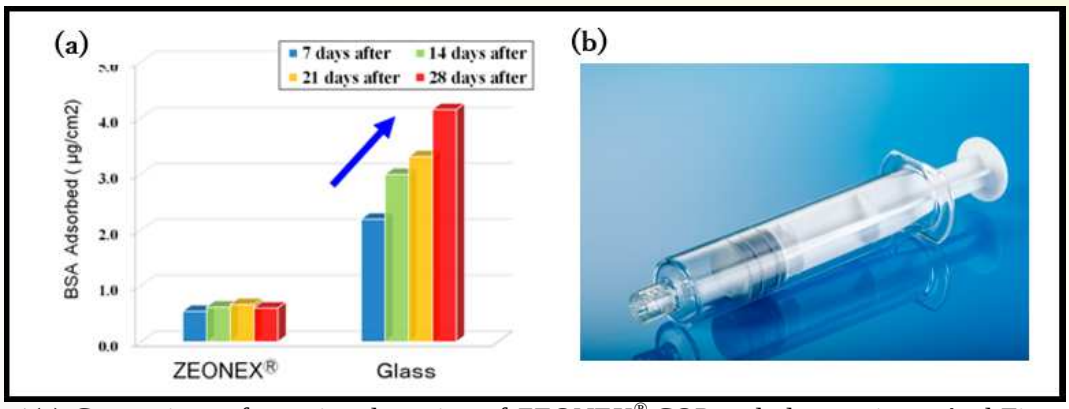

Figure 1(a) Comparison of protein adsorption of ZEONEX® COP and glass syringe. And Figure 1(b) Pre filled syringe made by ZEONEX®(Both figures are taken from ZEON homepage http://www.zeon.co.jp/press_e/190712.html)

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IL-3

Global Healthcare Challenge of Drug Resistance: Moment of Truth and Future Prospects

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BogaR Laboratories, Peddapuram-533437, E.G. Dt., A.P., INDIA

Abstract: Drug-resistant diseases such as antibacterial, antimicrobial, antifungal, and so on are commonly recognized as a global healthcare problem and estimated to kill ten million people annually by 2050. Apart from mortality, economic hardship is another major concern for drug resistance forcing 24 million people into extreme poverty by the year 2030. Therefore, drug resistance is becoming an alarming threat to global community in every year, and the developed super-bugs have no treatment to most of the existing drugs. Several strains of methicillin-resistant *Staphylococcus aureus* (MRSA), multi-drug resistant *Acinetobacter baumannii*, and *tuberculosis* (MDR-TB), and others have emerged as riskier and untreatable with existing drugs and new approaches are highly necessitated to discover powerful and smart drugs.

The moment of truth on developing such drug resistance and mechanisms of underlying such resistance poses to several explanations. It is time for us to question ourselves that why the drug resistance is happening at first place, and whether it is caused by human-made or evolutionary development and all together. Most of the drug-resistant diseases are due to unnecessary and widespread overuse of antibiotics/drugs, pollution, and other life-style changes by humans. Even cigarette smoke exposure develops significant resistance to the drugs for *S.Aureus* and it is better recognized such patterns now than the later and the ramifications are severe in the future that either ignored or missed to treat drug-resistant diseases. On the other hand, evolutionary development of drug resistance is still murky and there is no clear evidence as such to claim in confidence. However, thorough understanding of epigenetics and evolutionary process could find the clues to selected population where such prevalence of drug resistance and identifies the selection over genotype versus phenotype. Majority of the explanations on drug resistance are associated with human-made and that could trigger faster pace to influence the evolutionary process.

To overcome such drug resistance, new approaches of developing antibiotics are essential and robust antibacterial pipeline are necessary with new class of molecules. Importantly, we must promote good medical guidelines of identifying the bacterial infections and avoid excess usage of antibiotics, and stringent regulatory on quality of the drugs. Additionally, new development of antibacterial(s) thatare smarter than the bacteria and minimize the resistance by designing with hybrid functions of drug candidates and some of the recent research efforts on overcoming efflux of the drug, and other concepts will be discussed in the presentation.

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2. Agarwal, B., Karthikeyan, R., Gayathri, P., RameshBabu, B., Ahmed, G., Jagannadham, M.V.: “Studies on the mechanism of multidrug resistance *Acinetobacter baumannii* by proteomic analysis of the outer membrane vesicles of the bacterium”, *J. Proteins Proteomics*, 10, 1-15 (2019)

IL-4

Novel Diaminoquinazolines (DAQs) as an effective inhibitor of M. Tuberculosis, and a potential drug candidate for treatment of Tuberculosis (TB)

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Abstract: Tuberculosis (TB), an infectious disease caused by the bacillus Mycobacterium tuberculosis (Mtb), poses a major threat to public health. In its most recent report, the World Health Organization (WHO) has mentioned that TB is one of the top 10 causes of death worldwide. In 2018, 10 million people fell ill with TB, and 1.5 million died from the disease (including 251 000 among people with HIV). TB is a leading killer of HIV-positive people.Furthermore, TB, like other bacterial diseases, is confronted by problems of emerging drug resistance, which places an enormous strain on the public healthcare system [1]. In addition, billionsof people harbor latent infections with no clinical symptoms, butwith the potential to advance to active form. Current TB treatmentrequires a combination of four drugs, isoniazid (INH), rifampicin(RIF), pyrazinamide (PZA), ethambutol (ETH) for 2 months followedby an additional 4 months of INH and RIF. These drugs havebeen in use for many decades, contributing to a rise in the emergenceof multidrug resistant (MDR) and extensively drug-resistant(XDR) strains of M. tuberculosis and hence new drugs are needed urgently. 2,4-diaminoquinazoline class of compounds has previously been identified as an anti TB agents, keeping this fact in mind we conducted an extensive evaluation of the **DAQ**sseries for its potential asa lead candidate for tuberculosis drug discovery. Three segments of the representative moleculeN-(4-benzyl)-2-(piperidin-1-yl)quinazolin-4-amine were examined systematically to explorestructure–activity relationships influencing potency[2].

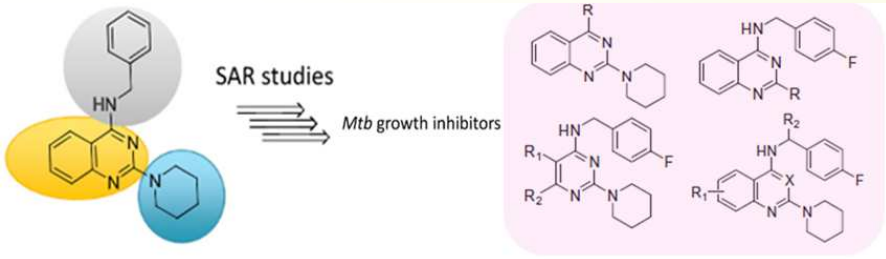

Figure 1: Synthesis of evaluation of substituted DAQ derivatives as anti-TB agent

References:

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IL-5

Design, Synthesis and Biological Evaluation of Small Molecules targeting Histone Deacetylase Inhibitors (HDAC) as Anti-Cancer Agents

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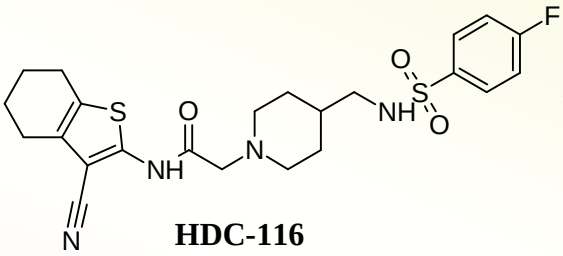
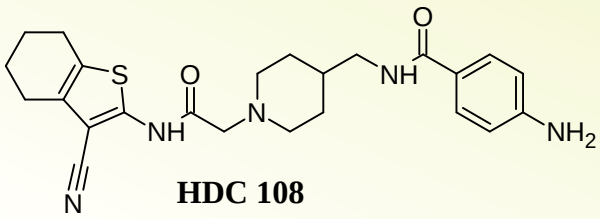
Abstract: This research majorly focused on the lead development for the selective inhibition of Histone deacetylase enzyme widely known as HDAC inhibitors. The main purpose is to design selective HDAC inhibitor as there are no known inhibitor which selectively inhibit particular isoform of HDAC because pan inhibitor have numerous side effect i.e tissue dependence, ineffective against solid tumor. HDAC divided in major 4 class and further subdivided in different isoform. Current research mainly targets the class -I specific inhibitor. In the present study, a series of novel histone deacetylase (HDAC) inhibitors using the tetrahydro-1-benzothiophene (1) as the capping group were designed and synthesized. HDC-116 and HDC-108 inhibits HDAC nearly 94% at 10 µM.

Keyword: Histone, HDAC, Benzothiophene



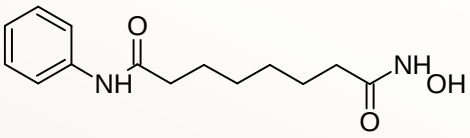
HDC-116

HDAC inhibition: ~95% at 10 µM



HDC 108

HDAC inhibition: ~94% at 10 µM



VORINOSTAT

HDAC inhibition: ~68% at 10 µM

IL-6

A Molecular Rotor Possessing a Cl-Pd-Cl "Spoke" on a Se-Pd-Se "Axle": Efficient Catalyst for Regioselective C-5Arylation of Imidazoles

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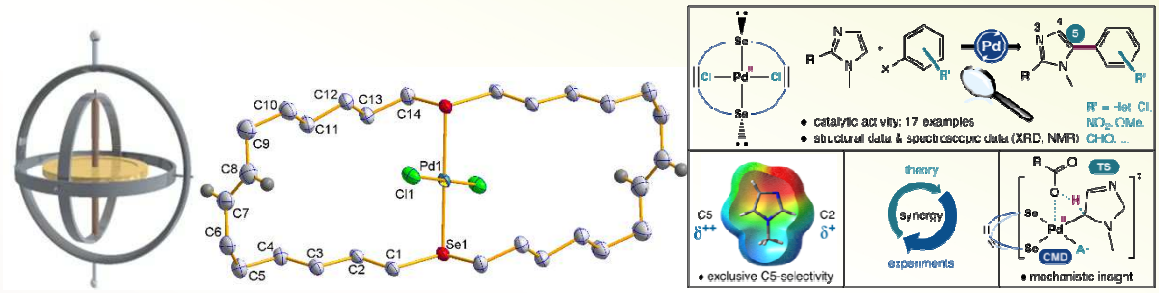
Abstract: New classes of robust air- and moisture- stable molecular rotor, whichcontain a palladium metal center encased by two selenium-anchored methylene linkers have been designed. These rotor molecules haveshown unprecedented catalytic performance in the arylation of imidazoles, *and* with exclusive C5-selectivity. This, to ourknowledge, is the first demonstration of the use of a molecular rotor in a highly regioselective catalytic reaction. The arylation ofimidazoles is an important reaction as it affords products which are commonly used in pharmaceutical applications, however, thecompeting C4 or C2-arylation often hampers the reaction. We shown that a palladium-based molecular rotor catalyst with the formula*trans*-($PdCl_2(Se((CH_2)_6CH{=}CH(CH_2)_6)_2Se)$) overcome this selectivity problem. This catalyst operates under open air with milderreaction conditions compared to existing palladium catalysts, which coupled with its exclusive C5-selectivy, supersedes otherprotocols to date. The intriguing function of this catalyst was studied using computational and experimental (XRD, VT-NMR)methods providing a plausible mechanism. Overall, this work shows a promising outlook for the use of molecular rotors in catalysisto enable unique selectivity paradigms using mild reaction conditions.



(a) (b) (c)

Figure 1. (a) Structure of a molecular rotor (b) Crystal structure of designed molecular rotor (c) Reaction under investigation and mechanistic insights.

IL-7

Are DDR kinases Druggable? : Our journey towards Cancer therapeutics

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Abstract: Cancer is considered to be a major killer globally. One of the causes is the deregulation of the kinase a primary mechanism by which cancer cells evade normal physiological constraints on the growth and survival. Such aberrant functions of the kinases in a cancer cell have highlighted them as one of the most successful families of drug targets. Innovative approaches in chemical biology have played a key role in validating the importance of kinases as molecular targets. Understanding crosstalk between intrinsic drug resistance mechanism relating to DNA Damage Response (DDR) and extrinsic resistance mechanism will enable the design of better therapeutic strategies, including combinatorial inhibition of kinases involved in DDR pathways to overcome chemo-resistance and improve therapeutic index of cancer. My talk would reflect the recent developments in the discovery of small molecules towards the most important kinases that are part of DNA damage and repair (DDR) pathway such as ATR, ATM and TLK developed in our lab.

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IL-8

Transforming Drug Discovery with Advanced Computational Modeling

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Abstract: Today computational techniques play a critical role in pharma R & D. Thanks to recent advancements in understanding the biology, growth in vast amount of Protein Structures, which led to developments in Structure-based drug design. Computational techniques are widely adopted in understanding the structure function relationship and for screening millions of molecules for lead identification and optimization. In the recent years many techniques has emerged in docking methods, binding energy prediction methods, Understanding the thermodynamics behind protein ligand interaction and in modeling the proteins etc. My talk highlights on these recent developments in computational methods and a case study on how these computational techniques helped in narrowing down to a few hundred molecules from database of millions of compounds. How we selected the leads, how we expanded from few molecules to millions of potential analogs using virtual combinatorial methods. The presentation also covers on lead optimized methods and designing selective molecules towards their target.

IL-9

Antiepileptic Drugs and Ketogenic Diet: An Uncanny Alliance to Bone

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Abstract: For more than five decades,antiepileptic drugs (AEDs) have been known to cause serious adverse effectson bone mineral density. AED therapy causes multipleabnormalities in bone metabolism, varying fromincreased bone turnover to osteopenia/osteoporosis and to osteomalacic disorder. Gross malformations in the bones allied mainly, but not solely, withthe cytochrome P450-inducing AEDs and these mayact as an add-on to risk factors for fractures in persons with epilepsy.In our lab, we have focused on developing models to study AEDs-induced changes in bone in rodent models. Our results provided evidence for several alternative mechanisms including deprived oestrogen levels, hyperhomocysteinemia, *Wnt* pathway inhibition etc.responsible for bone loss and suggested anti-osteoporotic agents that can be prescribed safely along with AEDs.The uncanny alliance of AED treatment was seen with not only conventional drugs like phenytoin, carbamazepine and valproate but also with some second-generation drugs. Further, the adverse effects on bone following AEDs were found to be more pronounced in ovariectomised animals. Recently, we observed the negative effects of MCT ketogenic diet on bone in experimental animals and suggested closer monitoring in vulnerable groups to evade long-term adverse effects. The choice of the AED treatment and the correct supplementation initiated at the right timecan shield the bony skeleton. We propose research to be carried out beyond the conventional supplementation of vitamin D and calcium for prevention and treatment of AED-associated deleterious effects on bone.

IL-10

The Most Poisonous Poison as a Model to Reframe Biology, Chemistry, and Physics of Evolution

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Abstract:

Background: Botulinum neurotoxins (BoNTs) as food poisons are the most poisonous poison known to mankind today. Among the unique traits ofthe seven serotypes (A-G) BoNTsits potency (being the highest amongst the toxins known) and longevity in a foreign cell place it way above any other reagents currently known. Other features include highly selective receptors on neuronal cells, a very novel zinc endopeptidase activity with very specific protein targets in SNARE proteins, and extremely selective cleavage sites. Are these features result of a tightly controlled evolution process of the *Clostridium botulinum*, an anaerobe of about 3 billion years? Genetic analysis of the seven serotypes, as well a series of BoNT like proteins found in non-clostridial bacterial and even non-bacterial species of the biological world provide evidence for their likely origin. However, their fundamental characteristics of targeting a process (exocytosis) by all seven BoNT serotypes, as well as some of the BoNT-like proteins, rather than a physical target, and surviving intracellularly for even 12 months inside a foreign cell are decipherable from the genetic diversity or evolution. Evolution is not only a reflection of change in the characteristic of biological species, but it is also related to diversity at every level, including species, individual organism, and even at the molecularlevel. Study of evolution in terms of molecular properties such as folding, flexibility, and dynamicsprovides us with another very unique and necessary dimension to examine molecular and sub-molecular mechanisms involved in the evolutionary process. Such information can be used todevelop countermeasures against botulism, and perhaps utility of highly evolved toxins as medicines.

Results: Genomic sequence analysis derived dendrogram has shown BoNT/C and BoNT/D at the root and BoNT/E at the terminal position. Assuming that all different serotypes of BoNT have evolved at the same mutation rate BoNT/E is the latest neurotoxin serotype because BoNT/E has the least sequence variation (highest conservation) in its cleavage site. Furthering this approach, we have examined protein sequence variations in BoNTs and their substrates, SNAP-25, and syntaxin using information entropy theory and bioinformatics tools. We have constructed the dendrograms and derived phylogenetic trees for all BoNTs and two of their three neuronal substrates (SNAP-25 and Syntaxin). We have also determined the frequencies of sequence variations at the cleavage sites of their neuronal substrate to examine the sequence entropy for each of the cleavage sites, which could shed light might their evolutionary development. We have further considered the protein structure of the optimally active form of the BoNT/A endopeptidase in the form of a molten globule that provides molecular flexibility for adaptive feature as a critical evolutionary trait for the chemical survival of the protein. Molecular dynamics of such a flexible functional structure maybe the true force behind the evolutionary traits of the BoNT endopeptidase.

Conclusion: BoNT's genetic diversity producing several types of toxin protein all targeting a physiological process, co-evolution of the toxin with its intracellular biochemical target, and molecular dynamics of molten globule state of optimally active structure provide a very wide dynamic range in modern science to address fundamentals of evolution process using BoNT as a model.

The study was supported in part by grants from Maryada Foundation and National Institutes of Health.

IL-11

Efficient and Regioselective Functionalization of Quinolones

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Abstract: Quinolone subunits are ubiquitous in a vast array of biologically active compounds, including pharmaceuticals, medicine and agrochemicals [1]. In view of interesting biological applications of quinolones, many researchers have been continuing their efforts to functionalize the quinolone scaffold at different positions. In this context, recently we have demonstrated *N*-/*O*-arylation of quinolone under metal-free conditions [2]. Similarly, C-2 and C-3 arylation of quinolone have been unveiled by other groups either by using haloarenes or arylboronic acids under metal-catalyzed (such as Ru, Rh and Pd) conditions [3]. On the other hand, C−H functionalization has also rapidly gained acceptance in the recent past as an alternate key tactic in the construction drug like molecules. Metal-catalyzed site-selective arylation of unreactive C–H bonds is an area of great importance for the design of atom economical approaches leading to useful organic molecules. Employing directing group (DG) to functionalize at the less activated position is an alternative and efficient approach in which C-H bond is activated by metallacycle intermediates. However, metal coordination to DG can commandments the site-selectivity of unreactive C–H bond arylation [4]. Recently, diaryliodonium salts have been emerged as versatile arylating partner in coupling reactions due to their attractive and benign properties such stable solids, electrophilic, less toxic, highly reactive, and recyclability [5]. Due to noteworthy properties of quinolones and utilities of diaryliodonium salts, we have developed regioselective protocols for the functionalization of quinolones by utilizing diaryliodonium salts. Details about the synthetic strategies and mechanistic pathways will be discussed in the conference.

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IL-12

The Role of Omics in Personalised Medicine: A Review of Outcomes in Cardiovascular Diseases

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Abstract: Personalised medicine (PM)is considered as an emerging model that is expected totransform our current healthcare system. Personalised medicine (PM) is known by different names such as Precision Medicine or Pharmacodiagnostics, and Theranostics. In last two decades, there has been increase in study of proteome, transcriptome, and metabolome in health and disease for accurate diagnosis, rationalized treatment and monitoring of treatment. Collective use of these approaches of modern biology are called as '-omics'.Emerging technologies, devices, sensors, smartphones can now measure and collect real time data on blood pressure, heart rate and rhythm, oxygen saturation, and many more vital parameters. Collected information can be link with genomics, metabolomics, proteonomics and microbiomics to discover pathogenesis at sub cellular level or to predict the risk healthy people. Therefore, integrated 'omics' approach can be really used inpredictive, diagnostic, and prognosticbiomarkers in cardiovascular diseases. In the proposed talk, speaker will provide an overview on the current updates of PM in cardiovascular diseases. Speaker will also discuss the use of the various technologies and tools in PM and the opportunities and challenges that arise during use of these technologies in PM.

IL-13

Synthetic Exploration of Aza-oxyallyl Cation Towards Oxindoles and 1,4-Benzodiazepines

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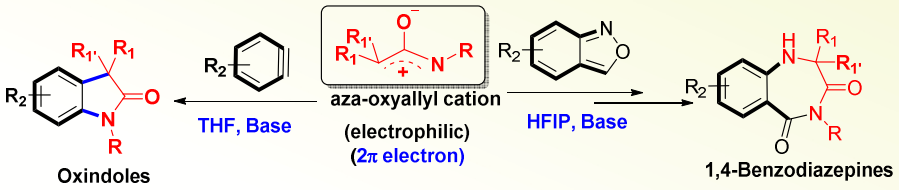
Abstract: Aza-oxyallyl cation have recently emerged as one of the prominent synthetic intermediate in organic synthesis. Since the seminal report of this intermediate in 1960's by Sheehan et al.,[1] it remained dormant for nearly five decades. It is only after the reports by Jeffery[2,3] and Wu,[4] who independently probed its utilization in 4+3 and 3+2 cycloadditions that the interest in aza-oxyallylcationwas rekindled. It serves as electrophilic 3-unit synthon and its utility has been demonstrated through various 3+m cycloadditions.Our own efforts in this area have culminated in efficient construction of oxindoles by using electrophilic arynes as 2-unit (2π electron)synthon. Thus, creating a unique opportunity for cycloaddition of two electrophilic species.[5] In another piece of work, we have demonstrated the adaptability of aza-oxyallylcationto act as single unit synthon, owing to extreme hydrogen bond donating ability of hexafluoroisopropyl alcohol (HFIP), resulting in active HFIP esters through multicomponent approach. The obtained HFIP esters were demonstrated to be facile intermediate for efficient construction of privileged Benzodiazepines.[6]



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IL-14

Arylidene-Rhodanine/Thiazolidinone Hybrids: Synthesis, Bioevaluation and Molecular Docking Study

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Abstract: Rhodanine plays an important role in the field of medicinal chemistry and drug discovery. The molecules with rhodanine scaffolds have possess various biological activities such as anticancer, antifungal, antitubercular, anticonvulsant, antiviral, anti-HIV, anti-inflammatory and antioxidant. Therefore, utilization of rhodanine scaffolds as building blocks must be applicable while drug designing. Another application of rhodanine is to be acts as Michael acceptor. Rhodanines are very easy to synthesize and among many derivatives of rhodanine, majority of bioactive rhodanines are 5-ene-rhodanines. They have also shows better pharmacological activities.[1] In recent years, most of the researchers show more interest in the designing and synthesis of rhodanine bearing therapeutic leads.

We have designed and synthesized highly functionalised arylidine-rhodanine/thiazolidinone conjugates and evaluated for their antitubercular as well as antifungal activities.[2] We have also performed the molecular docking, ADME predictions and will be discussed in the conference.

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IL-15

Molecular design, structural features of new RNA targeted antitumor metallodrugs for cancerchemotherapy

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Abstract: RNAs play critical roles in various biological processes and the dysregulation of long non-coding RNA targets was correlated with the stages and prognosis of several tumors. There is compelling rationale for the design of robust antitumor metallo-drugs that are largely targeted to non-coding RNAs(ncRNAs). The myriad binding of ligand scaffolds, modulating nature of metal ions at the target site along with the specificityof RNAs (i.e., site-specific recognition binding involving a uniqueRNA motif such as bulge sites) makes them an indispensable drug target. Molecular design of new RNA targeted chemotherapeutic metallodrugs was accomplished by using bioactive ligand pharmacophores along with some ancillary non-leaving diimines. Their structural features and pre-requirements of targeting RNA motifs will be discussed here.The drug candidates were found suitable for many phenotypes of cancers *viz*., breast (MCF–7), cervical (HeLa), prostate (PC-3), pancreatic (MIA–Pa–Ca–2), liver (HepG2) and kidney(A498) at a low intracellular concentration, thereby muting systemic toxicity issues. The results demonstrated that the metallodrugs could elegantly serve as a new class of RNA targeted chemotherapeutics and can lay a platform for interrupting crucial processes oftumorprogression.

IL-16

Bile acid Hybrids as Anticancer Agents

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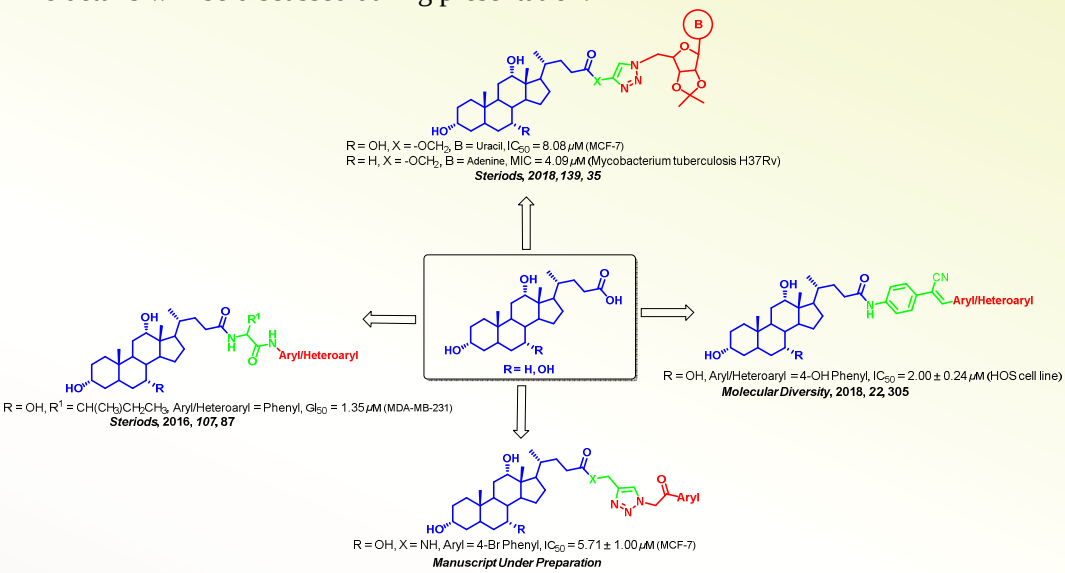
Bile acids (BA), the acidic sterols present in physiological enterohepatic circulation, possess a large, rigid, and curved (cyclopentano)perhydrophenanthreneskeleton structure possessing multiple hydroxyl groups on the steroid skeleton and a terminal carboxylic group. Bile acid science (Cholanology) has a history of more than a century, still the use of bile acid continue to evolve as one of the important supramolecular scaffold in medicinal chemistry and material science.[1]A number of bile acid derivatives have been found to induce apoptosis in many human cancer cells, such as prostate cancer cells, leukemic T cells, hepatocellular carcinoma cells, colon cancer cells, breast carcinoma cells, osteosarcoma cells, and cervical carcinoma cells.[2] Our group hasrecently designed and synthesized numerous series of bile acidhybrids and evaluated their potential as anticancer agent.[3]The details will be discussed during presentation.



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IL-17

Pd-CatalyzedAzide-Isocyanide Cross Coupling Reaction: Applications in Medicinal Chemistry and Bioimaging

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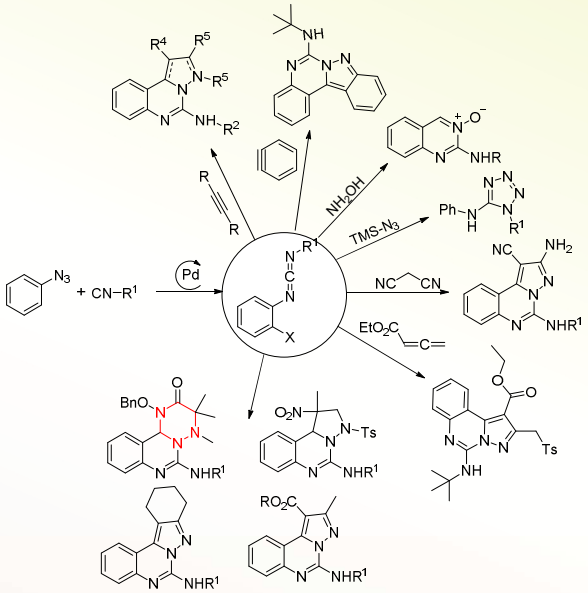
Abstract: We recently studied transition metal-catalyzedazide-isocyanide cross-coupling reaction in detail.[1] The study revealed that the transfer of nitrene, generated in situ from azide, on isocyanide is a concerted process rather than a two-step process involving a metallaaziridine intermediate as proposed in the literature. The study helped us to fine-tune an elegant method for the synthesis of carbodiimide, a versatile intermediate, in quantitative yield. Encouraged by the result, we devised a four-component reaction promoted by bimetallic relay catalysis for the synthesis of pyrazolo[1,5-*c*]quinozolines.[2] The tricyclic relay cascade involves the formation of five new chemical bonds and concatenation of six discrete chemical steps. Interestingly, pyrazolo[1,5-*c*]quinozolinesselectively inhibit EGFR, exhibit apoptosis throughthe ROS-induced mitochondrial-mediated pathway, and arrest thecell cycle at the G1 phase. The relay catalysis based on nitrene-transfer on isocyanide also provided rapid access to a variety of heterocycles that have application in medicinal chemistry and live-cell imaging.[3]



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IL-18

Sugars to Flavonoids and Other Molecules of Important Applications

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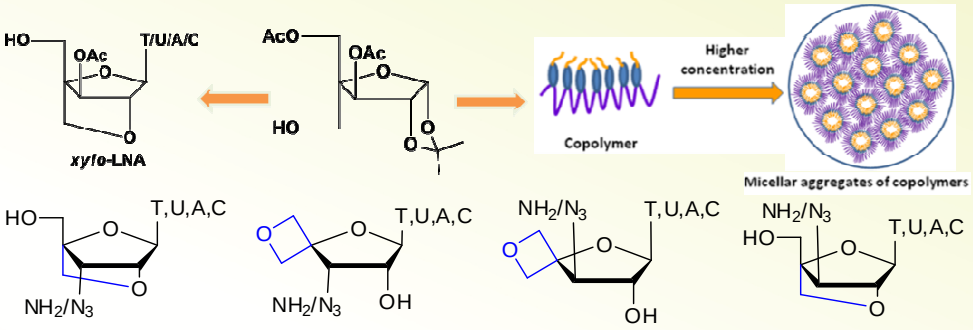
Abstract: The discovery of sugar modified nucleoside derivatives as potential antiviral agents and the emergence of antisense and antigene oligonucleotides as potential and selective inhibitors of gene expression have led to the considerable rise in the synthesis of modified nucleoside derivatives and nucleic acids involving them. Further, there has always been need to have biocompatible drug carriers capable of delivering water insoluble drugs with high transport and controlled release capacity.

We have developed an efficient biocatalytic methodology for the transformation of a trihydroxy sugar derivative obtained from glucose into novel sugar modified nucleosides and sugar-PEG co-polymer having application as drug delivery agents. Further, we have demonstrated for the first time that Chromanes can be synthesized from Glucose. Detailed results will be presented in the meeting.



Acknowledgements: We thank University of Delhi and Indo-German Science & Technology Center (IGSTC) for financial assistance.

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IL-19

Computational Studies on HSP90 inhibitors as possible anti-HIV agents.

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Abstract: A series of 2-isoxazole-3-yl-acetamide analogues were synthesized through novel intramolecular ring contraction as potential HSP90 inhibitors[1]. 6 compounds out of 15 derivates inhibited HIV-1 replication significantly at nontoxic concentration. The **2l** demonstrated high therapeutic index with highly conserved anti-HIV activity and it binds to the N-terminal ATP binding pocket of HSP90 and inhibits HIV-1 transcription in HSP90 dependent manner.

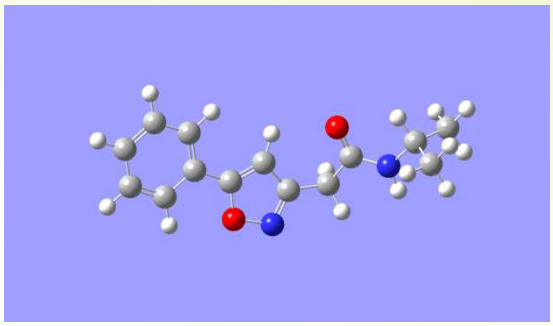

Fig1- **2l (**2-isoxazole-3-yl-acetamide analog**)**
CC_{50}=65.56 ± 2.48 µM
IC_{50}=39.48 ± 2.36 nM
TI= 1660.58

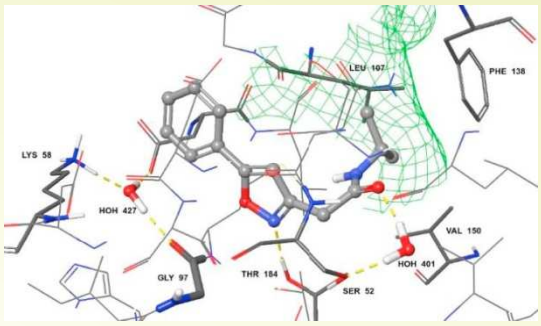

Fig2- Binding mode of **2l** with the active site of HSP90 showing hydrophilic interactions (hydrogen bonding as yellow dash line) of isoxazole ring and C=O of the amide with Ser52,and Thr184 through water bridge.

Density Functional Theory (DFT) calculation were carried out using the B3LYP method and 6-311G++(3d,2p) basis set in ground state. The SAR of a series of 2-isoxazole-3yl-acetamide analogues was derived and discussed to delineate HSP90 inhibition followed by anti-HIV activity.

Acknowledgment-Authors acknowledge to DST-SERB (EMR/2017/003331) for our financial support.

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IL-20

Transesterification/esterification reactions catalyzed by heterogeneous catalysts to form biofuel and fuel additives

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Abstract: The demand and cost of the biodiesel (BD) has been constantly increased over the past few years.[1] The production of global BD is expected to reach almost 39 billion litters by 2024, and accordingly the glycerol (GL) production, which is a by-product from BD, is bound to increase many fold. GL is considered as a nontoxic molecule having a variety of application in the synthesis of glycerol carbonate, glycerol monoacetate (GM), glycerol diacetate (GD) and glycerol triacetate (GT) etc.[2,3] The crude glycerol obtained from the biodiesel industry cannot be utilized directly for food and pharmaceutical industries due to its high contamination with methanol and the left out catalyst. Presently, triacetin and other molecules from GL are usually produced by the reactions in which homogeneous catalysts are employed.[4]Although these reactions yielded satisfactory conversion levels in short reaction duration, however, catalyst removal is mandatory which not only demand huge amount of water but also generate enormous quantity of industrial effluents. Moreover, literature reported heterogeneous catalysts demonstrated poor stability and moisture sensitivity and often led to the formation of a mixture of product.

In present study, mixed metal oxides, as heterogeneous catalysts,have been explored for the triglyceride transesterification to form biodiesel, andglycerol esterification to form the triacetin, and glycerol carbonate.

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IL-21

Orientated External Electric Field: An Invisible Catalyst in Bio(Chemical) Reaction

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Abstract: Oriented external electric field (OEEF) can be a remarkable catalyst in versatile chemical reaction e.g., C-H activation catalysed by synthetic metal-oxo compounds, nucleophilic substitution reactions, Diels-Alder reactions etc., [1-3]. Non-covalent interactions such as Anion-π, Cation-π, π-π, H-bonding or halogen bonding plays important contributing role in many biological phenomena e.g., conformation of protein and their dynamics can also be altered in presence of OEEF. Though, there are sufficient experimental[4] & computational efforts [1-3]on the aforesaid theme the idea yet to be well established. In this presentation, we will discuss effect of OEEF on two types of basic chemical reaction systems based on our preliminary model calculations and will further try to project the idea to define the real systems [5].

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IL-22

Experimental and theoretical investigation of ESIPT based Hydroxy-aryl benzimidazoles/Schiff bases as chromofluorescent sensor

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Abstract: Proton transfer is very fundamental process, occurs in a large variety of chemical reactions as well as in biological systems such as acid-base neutralization and enzymatic reactions. Excited state intramolecular proton transfer (ESIPT) is one studied experimentally and theoretically due to its applications in molecular fluorescence probes, luminescent materials, UV stabilizers, OLEDs and molecular logic gates. In general, the ESIPT process requires hydrogen bond between proton donor (–OH, $–NH_2$, or –NHR etc.) and proton acceptor groups (–C=O, –N= etc.), which must be at interacting distance to each other in a molecule. ESIPT process depends upon the distance of hydrogen bonding i.e. separation between the H-acceptor and donor atoms in molecule. The distance may change depending upon the ring size of system such as 5-membered, 6-membered or 7-membered.

In the present presentation, synthesis of various hydroxyl-aryl benzimidazoles/Schiff bases will be discussed for exploration of ESIPT phenomenon. These moieties exhibited excited enol and keto tautomeric emission bands.The presence of anions and metal ions has been realized by prohibiting ESIPT through coordination or deprotonation induced by metal and anions with ESIPT centres, resulting in detectable spectral change. Presence of substituent, extended conjugation on ESIPT centres further affects the keto enol tautomerism and thus fine tunes the emission channels. The stimuli induced bathochromic or hypsochromic shift of these normal and ESIPT based emission channels further open new emission channels and thus provided opportunity for simultaneous sensing of multiple analytes, biological interactions, miniaturization of logic gates

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IL-23

Cavity-enhanced absorption spectroscopy in gas and condensed phases: Applications to medical diagnosis

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Abstract: Cavity ring-down spectroscopy (CRDS), an optical cavity-enhanced absorption spectroscopy technique, directly measures the rate of absorption of light rather than the magnitude of absorption when the light is circulating in a high-finesse optical cavity. Because of its unique approaches, the ring-down technique readily offers 10 to 100 million times better detection sensitivity when it is compared with the traditional absorption spectroscopy techniques.

In this talk, I will discuss our latest developments of new-generation gas-phase ring-down spectroscopy techniques combined with the cutting-edge external-cavity quantum cascade lasers (EC-QCLs) operating in the mid-IR molecular fingerprint region [1,2,3]. I will talk about high-resolution fundamental molecular spectroscopy of numerous bio-medically relevant important molecules and their isotopic species such as $^{12}CH_4$, $^{13}CH_4$, $H_2{}^{32}S$, $H_2{}^{33}S$, $H_2{}^{34}S$, NH_3, NO and HDO exploiting the EC-QCL-based high-precision *cw*-CRDS technique. I will also talk about their ultra-sensitive detection and quantifications in a variety of environments such as in human exhaled breath with unprecedented sensitivity (in parts per billion, ppbv to parts per trillion, pptv levels) and high molecular selectivity.

Then, I will talk about how fundamental gas-phase CRDS spectroscopy can be employed in real-life applications in healthcare environments for *non-invasive* molecular diagnosis of diseases. I will particularly talk about our innovations and technology on the development of prototype breath analyzer [4] which can precisely and selectively diagnose stomach infection and ulcer disease by analyzing some unique panels of molecular species in human breath. The spectroscopic signature of the breath molecules, so called “breath-print” and the new prototype system will obviate painful endoscopy-based biopsy tests. The new device is now under the process of technology transfer (TOT) and subsequent commercialization. Finally, I will talk about some potential future directions of our work on gas-phase ring-down spectroscopy where new technology and products could be developed for societal applications.

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IL-24

Hantzsch Ester Mediated Reactions under Visible Light Irradiation

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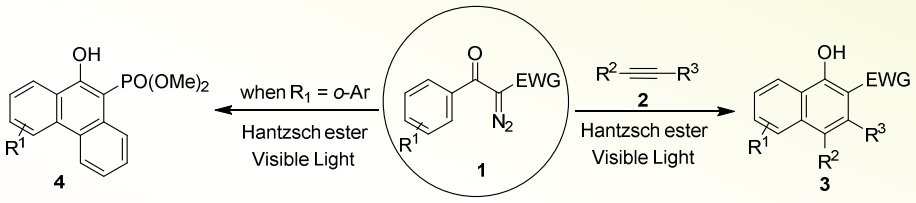
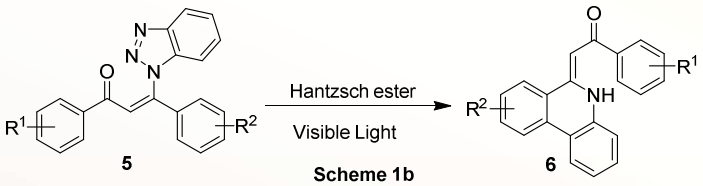
Abstract: Recently, the use of visible light to develop greener synthetic protocols has attracted the attention of the chemist's community and has led to the development of several useful protocols for C-C as well as C-heteroatom bond formation.[1]Although numerous reactions employing organic dyes as photocatalysts are known, numerous others use metal-polypyridyl complexes as photocatalysts. Since the use of metal photocatalysts defeats the very objective of developing "greener" reactions under visible light irradiation, the development of novel organic photocatalysts is highly desired.
The Hantzsch esters are known to be strong light harvesting molecules and good single electron as well as hydrogen atom donors upon visible light irradiation.These simple organic molecules can, therefore, mediate photoredox reactions with or without a suitable photocatalyst.[2]

Our group developed the Hatzsch ester mediated benzannulation of α-diazo phosphonates, sulfones and carboxylates **1**with alkynes **2**enabling direct access to the functionalized naphthalene-1-ol**3**.The strategy was extended to synthesize phosphorylated phenanthrene-1-ols**4** via intramolecular benzannulation of o-aryl α-diazophosphonates**(Scheme 1a)**.[3]We also developed Hantzsch ester mediateddenitrogenative intramolecular cyclization of benzotriazolyl chalcones **5** to access phenanthridine chalcones **6(Scheme 1b)**.[4]



EWG = $PO(OMe)_2$, SO_2Ph, CO_2Et

Scheme 1a



Scheme 1b

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IL-25

Palladium-CatalyzedSynthesis of Sulfur Heterocyclesand Their Biological Significance

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Abstract: Heterocyclic compounds containing sulfur constitute the structural motifs of a large number of pharmaceuticals, natural compounds, drugs, and agrochemicals and thereby sulfur heterocycles play a pivotal role in the field of new drug development. Gerhard Domagk achieved a Nobel Prize in 1935 for the first sulfa drug- prontosil rubrum. This discovery has given much importance to the synthesis of *S*-heterocycles as well as their chemical and biological behavior.Various powerful methodologies for their synthesis have been developed in recent decades. Among different influential methodologies, transition metal-catalyzed heteroannulation is explored as a useful and convenient method for the formation of *S*-heterocycles.Here, I will discuss on the use of palladium for the construction of various heterocyclic compounds with sulfur heteroatom. The presentation will focuson two main sections of *S*-heterocycles; the first one is “sultam” i.e. cyclic sulfonamide and the second one is “sultone” i.e. cyclic sulfonates through some recent examples from my research group.[1-6] There are also some review articles on “sultams” and ‘sultones’ from our research group. [7-9] The first part of my lecture will focus on the recent development of Pd-catalyzed synthesis of sultams and sultones and the second part will concentrate on the synthetic and biological applications of synthesized sultams and sultones in our laboratory.[10,11] The details will be presented in the conference.

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IL-26

Current Trends Leading to the Isolation of Novel Bioactive Lead Molecules for *Drug Discovery* from *Medicinal Plants*

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Abstract: Drug discovery is a multidimensional approach requiring several parameters of bioactive molecules such as safety, pharmacokinetics and efficacy to be evaluated during drug candidate selection. The lead molecules further subjected for lead optimizations by manipulating their structures in order to develop new and innovative drugs. Medicinal plants have played a vital role in health care form ancient times and they represent the rich resource of novel biologically active agents with diversified structural arrangements mainly in the zone where the worthy synthetic bioactive molecules do not exist. The remarkable number of recent drugs has been resulting from plants grounded for their traditional medicine value.The top most marketing drugs from the last century have been developed from natural products (Taxol from *T. brevifolia*, vincristine from *Vinca rosea* and morphine from *Papaver somniferum*, artemisinin from *Artemisia annua* etc.). During the end of twenty and beginning of 21st Century (1981-2002) 5% of the 1,031 new chemical entities accepted as drugs by the US Food and Drug Administration (FDA) were natural products and another 23% were natural-product derived compounds.Keeping in view importance of traditional medicinal plants in therapeutic area and continuous of our work to search the novel lead molecules from plants [1-4], recently, in our laboratory, we have isolated and identified the various lead molecules viz. novel spirostan saponins, anthraquinones, bis-iridoid glucosides, paederosides, and ursane-triterpenoids from traditional medicinal plants. In this presentation various compounds isolated in our laboratory and current trends leading to the isolation of novel bioactive lead molecules for *drug discovery* from *medicinal plants* will be discussed in detail.

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IL-27

Computational Identification of Antiretroviral Drug Candidates through Recognition of HIV(type 1) Conserved Glycoprotein Sequence

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Abstract: Antiretroviral drugs used in Highly Active Anti-Retroviral Therapy (HAART) starts inducing side-effects in HIV patients due to high mutation rate of HIV glycoprotein during prolonged period of treatment causing side effects - cancer and neurodegenerative diseases being most common in the list. The pipeline, prepared from data mining is made to identify the responsible genes for these side-effects during HAART therapy and two genes have been successfully identified. These genes can be studied during Drug Treatment in individual patients to predict the side-effects. With the help of computational tools, conserved sequences responsible for HIV entry on the glycoproteins have been identified. The conserved sequences in a variety of HIV virus strains of the Indian region, for specific target of the drug, have been shortlisted using immunoinformatics servers and tools. Affinity of entry inhibitor market drugs with the predicted sequences of protein structures can be checked using Molecular dynamics simulation program. A Computational model based on results of the binding investigations of market drugs and potential targets to recognize effective pharmacophore has been developed and new drug candidates for inhibition of HIV entry and fusion have been modelled.

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IL-28

Graphene Oxide Promoted a Novel Multicomponent Reaction for the Synthesis of 3-Substituted Quinazolinones Using DMSO as One Carbon Source

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Abstract: Quinazolinones, are extensively used in the fields of pharmaceutical, agrochemical and material sciences. Especially quinazolin-4(3H)-ones are an important class of compounds among N-heterocycles in organic chemistry, owing to their diverse range of biological and pharmacological activities [1,2] such as anticancer,[3] antihypertensive,[4] antitumor,[5] antituberculer[6] and antiinflammation[7] and so on.[8]

Herein, we report the synthesis of 3-substituted quinazolinone from commercially available isatoic anhydride, amines and DMSO as methyl source through a novel multicomponent reactions using graphene oxide as reusable catalyst. It is worth mentioning here that several methods for the synthesis of quinazolinones require metal catalyst and harsh reaction conditions, whereas our catalyst system provides these heterocycles using multicomponent reactions under recyclable catalyst. Synthesized graphene oxide was well characterized by scanning electron microscope (SEM), X-Ray Diffraction (XRD), energy dispersive X-ray (EDX) spectroscopy and X-ray Photoelectron Spectroscopy (XPS). A series of 3-substituted quinazolinone was developed under mild and eco-friendly conditions in moderate to good yields.[9]

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IL-29

Synthesis and spectroscopic characterization of some organic-inorganic hybrid complexes of organotin(IV) incorporating the anti-microbial activity analysis

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Abstract: Organic-inorganic hybrid complexes of organotin(IV) have received considerable attention in the past few decades. Important developments have been noticed in the structural characterization of these complexes owing to the use of advanced spectroscopic techniques. The structural features of organotin(IV) complexes have been correlated with their biological activities along with the investigation of structure-activity relationships. The nature and number of organic groups and donor atoms attached to the central tin atom, coordination number of the tin as well as other substituents like halogens also influence their activity. Organic-inorganic hybrid complexes of organotin(IV) are known for their anti-bacterial, anti-fungal, anti-tumor, insecticidal and cardiovascular properties. These complexes have also been used in the prominent field of catalysis, biotechnology, organic synthesis, etc.

Organotin(IV) is known to form a number of complexes with potential organic ligands having nitrogen, oxygen and sulphur donor atoms. These ligands can be sterically congested heterocyclic β-diketones, fluorinated/ non-flourinated β-diketones, N-protected aminoacids, Schiff's bases, etc. The organic-inorganic hybrid complexes of organotin(IV) show superior properties that is important for their industrial and biological utilizations. The anti-microbial activity of these organotin(IV) has increased on complexation with potential organic ligands.

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IL-30

Natural products-inspired discovery and development of novel antifungal and antibacterial agents

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Abstract: We have extensively worked on several plant species and isolated a large number of novel compounds belonging to different classes (alkaloids, polyphenols, steroids, amides, terpenoids, etc.). Several of these compounds have shown interesting biological activities, remarkable of them has been our extensive work on the development of compounds that lower PKC levels and suppress the ICAM-1 and VCAM-1 expression, and thus were found to be good anti-inflammatory & anti-asthmatic agents. Very recent studies have focused on the development of novel antimicrobial agents against various deadly fungal and bacterial infections, viz. against botulism and aspergillosis.

Details of these studies will be discussed at the ISCBC-2020 Conference.

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IL-31

Linear dicarbonyls as suitable substrates for amine catalyzed transformations: Synthesis of medium-sized *N*-heterocyclic compounds

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

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IL-32

A multifunctional therapeutic approach: design, synthesis and identification of novel multitarget–directed ligands against Alzheimer's disease

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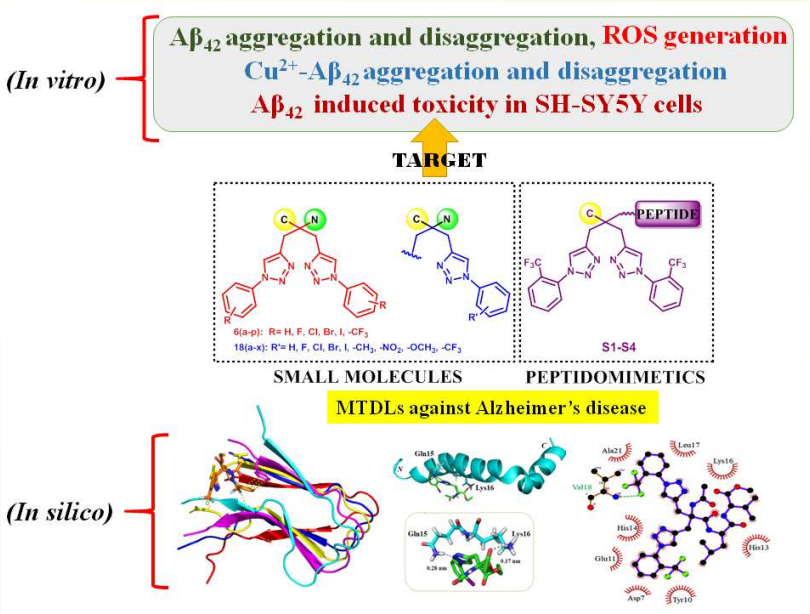
Abstract: Alzheimer's disease (AD) is a devastating neurodegenerative disorder and currently affects ~50 million people worldwide and this number is projected to increase to 152 million by 2050. The currently administered drugs for AD, manage symptoms and provide incomplete symptomatic relief. The lack of effective treatment, imminent increase of the socioeconomic impact of AD and large failure of drug candidates in clinical trials highlights the urgent necessity to identify new therapeutic agents. Taking into account the multifactorial pathology of AD, the multipronged approach is the key component in designing molecules as potent therapeutics[i]. In this regard, we carried out *in vitro* and *in silico* studies to identify novel triazole based scaffolds as multi–target–directed ligands (MTDLs) against AD[ii]. The triazole based compounds are designed to target four major AD hallmarks that include Aβ aggregation, metal–induced Aβaggregation, metal dys–homeostasis and oxidative stress. We have synthesised a library of mono-triazole, di-triazole based compounds and short modified peptides and evaluated their efficacies as potent MTDLs against AD. The designed triazole based scaffolds, possessing structural moieties capable of targeting multiple pathological causes of AD, could provide an efficacious drug candidates based on the multipronged approach.



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IL-33

Metal-Free Carbon-Sulfur and Phosphorus-Chalcogenides Bond Formations

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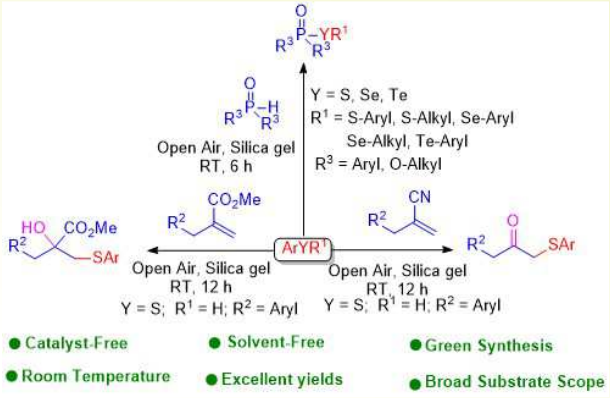
Abstract: Organic frameworks possessing chalcogenide and phosphorus moieties play an important role in organic synthesis, pharmaceuticals, materials, medicinal chemistry, and agrochemicals.[1] Traditionally, such molecules were synthesized *via* transition metal-catalyzed cross-coupling reactions. In recent years, the synthetic organic chemists are looking for suitable alternatives of traditional transition-metal catalysts for the synthesis of these molecules. This talk will cover the recent findings of metal-free C-S and P-Chalcogenide bond formations from our laboratory.[2]



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IL-34

Time gated Long-lifetime Lanthanide Luminescence to Study Dynamic Molecular Interactions with Improved Resolution

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Abstract: Capturing dynamic molecular interactions in living cells is challenging due to a number of reasons including low spatial and temporal resolution of the existing methods. Noise generated by the instrumentation setup used for detection of the signals as well as the auto-fluorescence of the cells diminish faint signals in commonly used techniques. Time-gated luminescence resonance energy transfer (LRET) microscopy with a selectively targeted, luminescent lanthanide protein labels afford improved speed and sensitivity over conventional energy transfer methods due to unique properties of lanthanide metals such as their long lifetime, large stoke shifts and characteristic narrow emission peaks. Moreover, a 6-fold difference was observed in the mean LRET signal from cells expressing interacting fusion proteins and from control cells expressing non-interacting mutants. The technique offers the possibility of multiplexed imaging.

IL-35

Development and Validation of Analytical Methods for drugs used in treatment of Alzheimer's (Memantine HCl) and Depression Disease (Nortriptyline HCl)

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Abstract: The chromatographic separation was achieved on C18 (250 × 4.5 mm, 5µ) column using isocratic mobile phase comprises of buffer (pH-5.2): methanol (40:60 v/v) pumped at a flow rate of 1.0 mL/min. The column effluents were monitored using RI detector. The retention time of MEM was found to be about 6.5±0.3 min. The detection of effluent was monitored using RI detector.

Result: The developed chromatographic method was validated and found to be linear over the concentration range of 5.0 - 45.0µg/mL for MEM. Mean recovery of MEM was found to be99.2±0.5%w/w. The method was found to be simple, fast, precise and accurate which can be utilized for the quantification of MEM in dissolution samples.

Conclusion: The proposed liquid chromatographic method provides simple, accurate and reproducible methodology for quantitative measurement of memantine hydrochloride in dissolution sample using refractive index detector without any interference from the excipients. The proposed method is very simple and can be used without derivatization of compound under analysis. This saves time and also reduces economic burden of laboratories.

The method validation results shows that the method is specific, stability indicating, precise, accurate and robust which can be utilized for the determination of assay of NortriptylineHCl in Nortriptyline tablets. The method is linear over the range of 50 - 150.0µg/ml drug concentration. This method can be used by any common laboratory for determination of Nortriptyline HCl in Nortriptyline tablets.

IL-36

Impact of Green matrix towards the Expansion of Miscellaneous Heterocyclic Scaffolds and their Biological significance

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Abstract: The impact of green matrix towards the expansion of miscellaneous heterocyclic scaffolds are the great challenge with multicomponent reactions (MCRs) protocol. Herein, we explore the significantmethodology for the augmentation of one-pot reactions for the Pyridone/quinazolinone and pyrimidinetrionederivatives using green matrix.The titled derivatives accomplishedover the formation of new C-C bonds, one C-N bond, whichcausescyclization in the final motif. The currentpractice works efficiently, without affecting sensitive functionality in the reactants, simple operational procedure, provide excellent reaction yield in short time, use of recyclable catalyst.The mounting interest for synthesized scaffolds has led to increasetheir courtesy towards the pharmaceutical and medicinal interest.

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IL-37

Organo and Photoredox Catalysis forC-C bond formation

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Abstract: Silyloxy furans, useful in accessing γ-butenolides and γ-lactone frameworks, have been extensively explored in the total synthesis of natural products and biologically active molecules. These heterocyclesare well known as a vinylogous nucleophile and after reaction with carbonyl and carbonyl derived compounds (aldehydes, ketones, aldimines, ketimines, enals, enones, and heteroatom-stabilized carbenium ions) offer a multitude of highly functionalized structures.[1],[2],[3]However, methodologies utilizing a vinylogous nucleophile are still limited and many important reactions are still unexplored. In this talk, a highly diastereo- and enantioselectiveorgano catalytic asymmetric vinylogousMukaiyama-Michael addition of various silyoxyfurans to enones,[4] and vinylogousaldol reaction of 2-silyloxyindoles to ketones, which proceeds through the bifunctional catalysis,[5] will be presented. Highly regio- and diastereo- selective Lewis acid catalyzedvinylogousnucleophilic substitution reaction with diarylmethanols will also be highlighted.[6]While thereactions demonstrated here are unprecedented examples of expanding the scope of these excellent vinylogous nucleophiles there still remains many reactions and substrates that do not have practical reactivity with either a Lewis or an organocatalyst and require an alternative strategy.

Photoredox catalysis has gained significant importance for the construction of a wide variety of non-traditional bond in the past few years. In fact, Coumarins, a phytochemical with wide spectrum of bioactivities have become an extremely attractive molecule. Here, a photo-induced decarboxylative 4-position alkylation of coumarins will be discussed. Photo-induced single electron transfer has been initiated by utilizing the visible-light absorptivity of Eosin Y for a reductive generation of alkyl radicals from N-(acyloxy)phthalimide esters.[7] Depending on the nature of N-(acyloxy)phthalimide esters (primary, secondary, and tertiary carboxylic acid derived) several saturated and unsaturated C-4 alkylated coumarins were synthesized. Both control experiments and photophysical studies supported a radical based mechanism for the selective alkylation. Another cross-coupling of alkylpyridinium salts and coumarins has also been developed. Both primary and secondary alkylpyridinium salts can be used, and high functional group and heterocycle tolerance is observed. Mechanistic studies indicate the formation of an alkyl radical, and controlling its fate was key to the success of this reaction.[8]

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IL-38

Stereoselective Synthesis of Natural Product Inspired New Bioactive Glycohydrids

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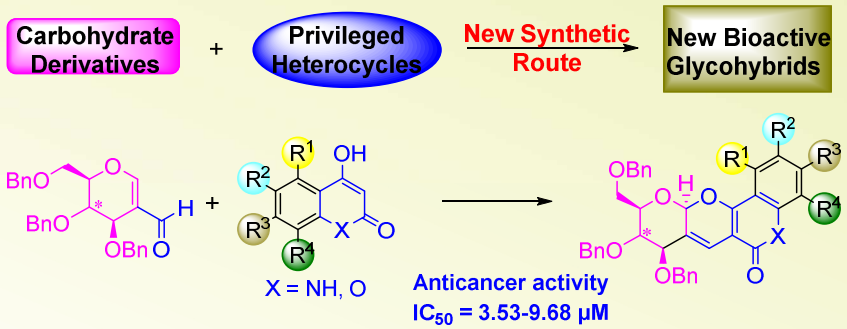

Abstract: Construction of drug like molecules is a challenging task in drug discovery process. Pyrano[3,2-c] -quinolones and -pyranones structural motifs are commonly found in natural products with diverse biological activities. As part of a research programme aimed at developing efficient synthesis of natural products like small molecules, we designed and developed facile stereoselective synthesis of two series of carbohydrate fused pyrano[3,2-c]-quinolone (n = 23) and -pyranone (n = 22) derivatives starting from 2-*C*–formyl galycalsreacting with various 4-hydroxyquinolones and 4-hydroxycoumarins respectively in shorter reaction time (15-20 min). Antiproliferative activity of these synthesized carbohybrids were determined against MCF-7 (breast) and HepG2 (liver) cancer cells. The selected library members displayed low micromolar (3.53-9.68 µM) and selective antiproliferative activity.[1-2]We have also developed a new route for the preparation of chirally enriched tetrahydrocarbazolones and tetrahydrocarbazoles,[3] and carbohydrate based organogelators.[4]The details of these findings will be presented therein.

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IL-39

GREEN NANO MATERIALS FOR SUSTAINABILITY

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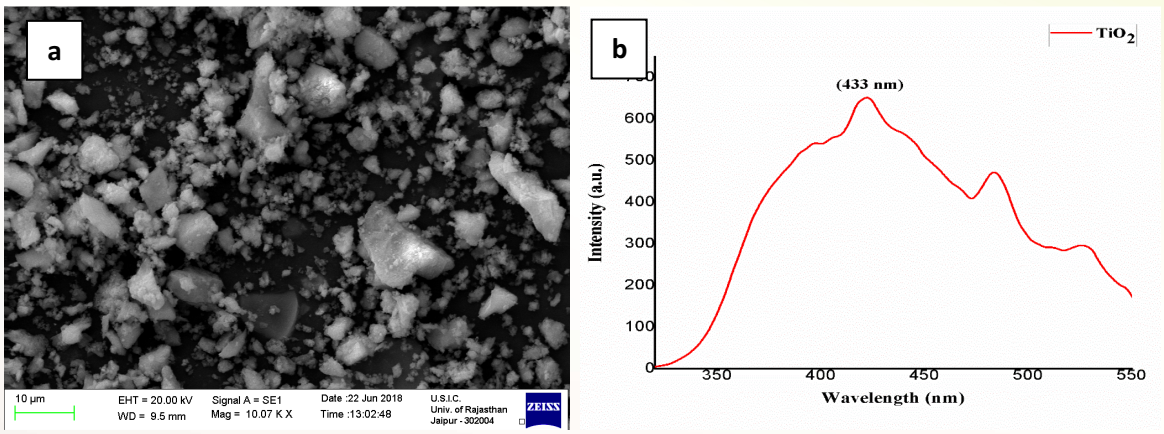
Abstract: Advances in nanomaterials synthesis, integration into devices, and characterization, along with modeling and understanding of nanoscale physical phenomena have all contributed to significant accomplishments in these areas. Green fabrication of nano materials is carried out by employing reducing and stabilizing agents from natural resources. It does not involve the use of toxic chemicals and hence it is a greener, safer, and environmentally sustainable route for nanomaterials synthesis. Moreover, the strict environmental legislations consideration has lead to develop *greener route*s which are significantly efficient for the synthesis of nanomaterials/nanoparticles. Nanostructured metal dioxide and metal oxide NPs/graphite oxide composites were fabricated via *greener* approach. Low cost hypoallergenic material were developed using *green* nanomaterials. Metal oxide nanocomposite core shell fabricated for the removal of the dyes from effluents and/heavy metal ions from aqueous solutions/water, thereby, making it potable. Likewise, *green* nanocomposites were tested to reduce lead toxicity in soldering wires and also benefit the microelectronics packaging and assembly industry. The fabricated *green* nanoparticles/nanocomposites were characterized by employing standard tools and techniques, viz., UV-vis spectrophotometry (UV), FL spectroscopy (FL), FT-IR spectroscopy (FT-IR), SEM, XRD, etc. These innovative nano-materials have multifold utility in numerous sectors such as environmental detoxification, health-care, pharmaceutical, metal and material industries, etc.

Keywords: *Green n*anomaterials/nanocomposites, eco-sustainability, SEM, XRD.



Figs.: (a) SEM image of CeNPs and (b) Fluorescence Spectra of TiO_2 NPs

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IL-40

Role of Elsevier Life Science Solutions in Drug Discovery Process

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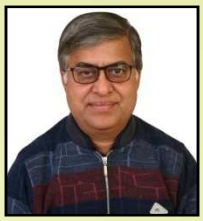
Abstract: At Elsevier Life Sciences, we share a common purpose with our customers – to accelerate science to improve health. Elsevier enables R&D productivity through our unique expertise in curating, enriching, integrating & harmonizing scientific datasets.

We already know that we are helping improve life expectancy across the globe by producing highly efficacious and safe drugs. But this also implies that the new drugs that are brought to the market need to be significantly better than the ones that already exist or treat an unmet disease. Numerous people have articulated the challenges of drug discovery. And when we zoom in to just consider the day-to-day challenges of a researchers this becomes apparent. Early drug discovery requires a multi-parameter approach - we are often trying optimise a multitude of parameters to create a good drug candidate. In reality, we are often jumping from one parameter to another. But when the volume of information in so vast, how do researchers cope? Do they succumb to the “Impending data lake of doom”. And even if they survive that stifling challenge, one still have the task of understanding and connecting the information together in a productive way. But on the other hand, if we restrict ourselves to what we know we can lack creativity.

Within our solutions suite we try to assist researchers by extracting and normalising data coming from large volumes of relevant documents (literature and patents). We try to deliver this in a user friendly and actionable way and I think we do a pretty decent job. We are working on the project that will leverage the data in our product to create predictive capabilities to strengthen across this drug design cycle. What we do strongly believe is that high quality data will make a difference and we hope to prove that by putting these solutions into the hands of our users as soon as possible.

IL-41

An Innovation Process and Concerns of Green Chemistry: Natural-product-inspired Pot-economy Synthesis of Small Molecules of Biological and Industrial Relevance



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Abstract: Nature is an irrefutable source of inspiration for the discovery and development of potent biologically active compounds.Several small molecules of natural origin including polyphenolics and indole based heterocyclic compounds have drawn great interest from the scientific community as they are associated with wide range of biological activities including antimalarial,anticancer, antibacterial, antifungalandanti-inflammatory etc. However, exploration of these molecules is severely hindered by their insufficient percentage in their natural resources, difficult isolation procedure, limiting trials for wider applications besides their tedious synthesis involving protection-deprotection strategy.The shortcomings of the prevalent methodologies have provided a fresh stimulus to develop a strategy based on Green Chemistry with minimum number of steps, atom economy and waste minimization besides being devoid of protection-deprotection steps. Our group from noticeable time has been working on such green methodologies for synthesis of various phenolic based bioactive molecules like FEMA-GRAS approved 4-vinylphenols, stilbenoids (symmetrical/ unsymmetrical, distyrylbenzene and octupolar stilbenes) and stilbene-chalcones/stilbene-cinnamate hybrids and their biological evaluation. Very recently,our group have developed a pot-economy synthesis of salvionalic acid mimicking molecules which have shown superior antagonistic profiles against the glioma C6 cell line that causes one of the most lethal and malignant forms of brain tumors. The details ofsynthetic protocol, biological and industrial relevance of natural and non-natural phenolic compounds and indole based heterocyclic compounds will be discussed during presentation.

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IL-42

Development of green methodologies in organic synthesis

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Abstract: Green chemistry is a new way at looking organic synthesis since it offers better environmental and economic advantages over the traditional organic synthesis.[1] In recent years, various methods have been developedin both academia and industryto archive the goals of green chemistry included the replacement of organic solvents by green solvents and use of biocatalysts in place of metal catalysts [2,3]. In this context, we have developed a first biocatalyticaza-Michael addition reaction of less nucleophilic aromatic amines to enones. Moreover, a highly efficient and green approach for the synthesis of γ- keto/nitrile sulfones using N-sulfonylhydrazones and enones/acrylonitrile in water has been developed. We have used water as a mediator in the absence of any base or catalyst to decompose N-sulfonylhydrazones to use as a sulfonyl-transferring reagent in the selective sulfa-Michael reaction.

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IL-43

Strategies to Engage Undergraduates in Meaningful STEM Research

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Abstract: It is essential for any nationto produce a pool of highly talented scientists to be a global leader in scientific discovery and innovation. To ensure that a nation produces sufficient PhDs in science, technology, engineering and math (STEM) field, it becomes urgent to recruit and retain young generation in STEM discipline and motivate them to peruse doctorate programs. To achieve this goal, one of the evidence based strategy is to engage undergraduate students in meaningful research leading to publications in peer-reviewed journals and presentations at scholarly meetings. My current research at University of Houston-Downtown (UHD), a four-year undergraduate institution,engages undergraduates in the area of cancer drug development and phage therapy. My lab has investigated hundreds of synthetic compounds for their anti-cell proliferative properties. As part of a national project, my lab also works on isolating and characterizing novel phages that can be used to treat bacterial infections. My students have isolated more than 50 phages in few years. Both projects have resulted in multiple publications in peer-reviewed journals and students have entered into doctoral programs.

IL-44

Computational screeningof potential inhibitors against β_2m aggregation in Dialysis-related amyloidosis

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Abstract: The misfolding of β_2-microglobulin (β_2m)leads to amyloid fibril deposition mainly in the skeletal joints in dialysis-related amyloidosis (DRA)[1]. The identification and characterization of small-molecules that bind β_2m and possibly inhibit its aggregation remain unexplored. Continuing with our focus on the computational investigation of the molecular mechanism of protein-aggregation derived diseases [2], a combined ligand-based virtual screening approach and molecular dynamics (MD) simulations were employed to explore potent small-molecule inhibitors against β_2m aggregation in the present study (Fig. 1) [3]. The ligand-based virtual screening approach using rifamycin SV (RSV) as a reference compound was employed to screen compounds from various small-molecule databases. Woods et al. reported RSV as a potent inhibitor of β_2m aggregation [4]. The lead compounds with a higher binding affinity than RSV were filtered from a library of ~800 compounds using molecular docking. Three compounds, ChEBI68321 (C_1), ChEMBL360190 (C_2), and ZINC3091144 (C_3), displaying excellent binding free energies of –51.29, –36.51, and –34.36 kcal/mol, respectively, with β_2m were subjected to MD simulations to get insights into the binding locations, key interactions and structural stability of the β_2m–ligand complexes.The hydrogen bond analysis depict higher structural stability and reduced flexibility of the loop regions of β_2m in the presence of C_1, C_2, and C_3. The *in silico* guided approach employed in the present study have identified promising lead compounds against β_2m aggregation in DRA.

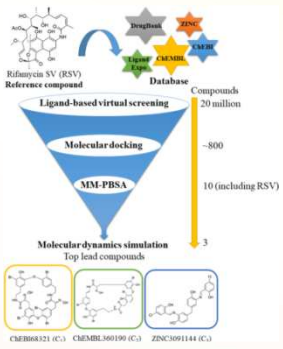

Fig. 1: The flowchart of the integrated computational methodology employed to identify potential inhibitors against β_2m aggregation in Dialysis-related amyloidosis.

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IL-45

Synthesis of various carbocycles and heterocycles from functionalized benzyl cyanide

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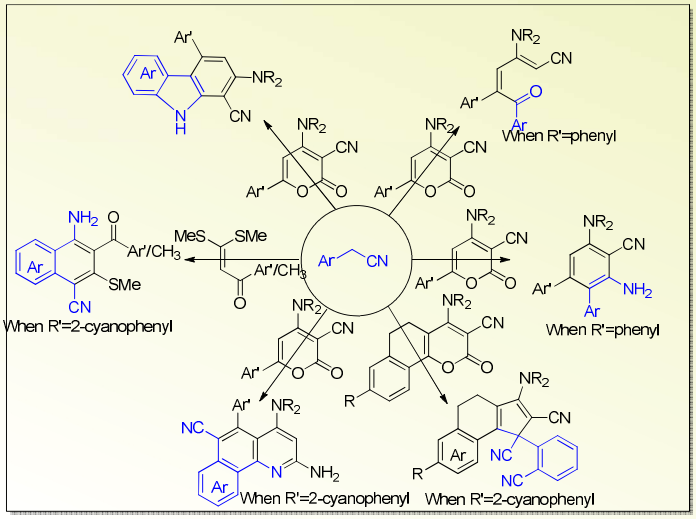
ABSTRACT:



Various functionalized benzyl cyanides were used as precursor from several decades. Recently, we have explored the functionalized benzyl cyanide as a carbanion source for various reactions. We studied 2-cyanomethylbenzonitrile, benzyl cyanide and o-and p-substituted benzyl cyanide and used them as a carbanion source to explore their chemistry. Various functionalized naphthalenes was afforded in good to excellent yield by reactions of ketenedithioacetals with 2-cyanomethylbenzonitrile.[1,2] Furthermore, 2-cyanomethylbenzonitrile provides highly functionalized beno[*h*]quinolines by ring transformation with 2-pyranone.[3] In addition, use of 5,6-dihydro-2*H*-benzo[*h*]chromene provides 4,5-dihydro-1*H*-benz[*e*]indenes.[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 functionalized benzyl cyanide as carbanion source to carry out the ring transformation of 2-pyranone and various teraryls and enones has been achieved under different reaction conditions.

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IL-46

Carbon disulfide: Greener syntheses for biologically potent scaffolds

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Abstract: Structurally diverse organosulfur compounds displayed plethora of important applications such as pharmaceuticals, agrochemicals, intermediates in organic synthesis and also has been employed as a useful synthons for the generation of structurally diverse biologically potent scaffolds.[1] Many of them have been approved as drugs, prodrugs and drug candidates. Keeping the view of importance of these compounds, extensive efforts have been made by the scientists around the globe to generate various kinds of structurally diverse organosulfur compounds from simple to the complex molecules employing traditional methodologies such as use of thiophosgene and its derivatives, which are harmful reagents. In recent years, carbon disulfide has been emerged as a cheap and safe alternative to generate various kinds of structurally diverse biologically potent organosulfur scaffolds employing various kinds of reagents and catalytic systems. In the present talk,[2] I would like to discuss some of our recently reported novel and efficient synthetic methodologies for the synthesis of acyclic biologically potent organosulfur scaffolds such as dithiocarbamates, trithiocarbonates, dithiocarbazates etc., employing carbon disulfide and a variety of reagents and catalytic systems.

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IL-47

Abstract Awaited

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IL-48

Development of Chiral catalysts for Asymmetric Organic Reactions

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Abstract: The optically active compounds have various applications including pharmaceuticals, agricultural chemicals, flavours, fragrances and material.[1,2]Asymmetric catalysis is important tool for the synthesis enantio- and diastereo- selective compounds. We are working on the development of organocatalysts as well as chiral metal complexes for asymmetric organic transformations. We have developed variety of (*L*)-Prolinamidesas catalysts for asymmetric aldol reaction between isatin and acetone, afforded 3-alkyl-3-hydroxyindolin-2-one as a product ingood yield and good*ee*.[3]We also modified MacMillan catalyst with imidazolium ionic liquid as a recoverable catalyst for the enantioselective Diels-Alder reaction.[4]

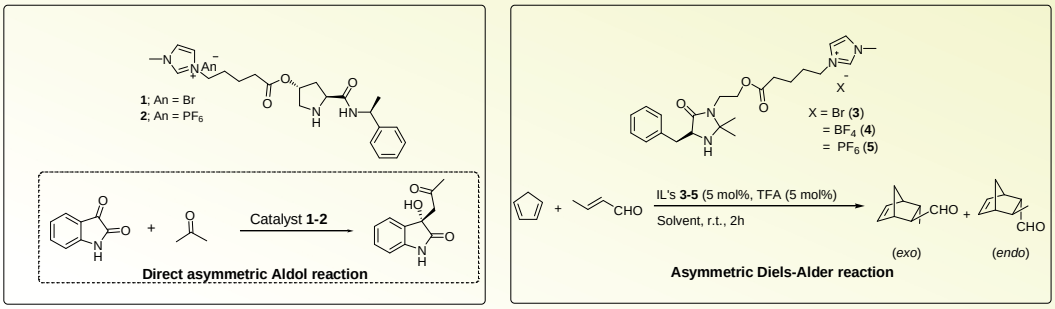
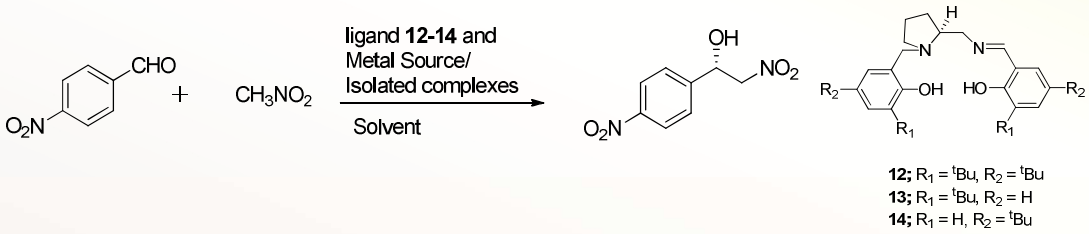


Figure 1: Catalysts for asymmetric Aldol and Diels-Alder reactions

We also developedSingle chiral center C_1 symmetric salalen ligands(**6-8**) were synthesized from (*S*)-proline and its Cu(II) and Mn(III) complexes were used as catalysts for the asymmetric Henry reaction between aromatic aldehydes and nitromethane/nitroethane (Scheme 1).[5]



Scheme 1: Asymmetric Henry reaction catalyzed by complexes of Cu(II) and Mn(III) of Salalen ligands

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IL-49

New Metal Based Pharmaceuticals, Structural Characterisation and their Anti-cancer activity

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Abstract: Molecular Drug design, synthesis and computation chemistry is an interdisciplinary thrust area of chemical biology research,development of new drug design and therapeutic strategies that could target cancer cells leaving normal cells unaffected still continues to be a challenge. Series of New pharmacophore of metallic compounds were designed, synthesized and characterized by various spectroscopic methods and further confirmed by X–ray crystallography. *In vitro* DNA binding studies of the compounds investigated by absorption and emission titration methods and docking studies with the DNA duplex. Gel electrophoretic assay demonstrates the ability of the compounds to cleave pBR322 DNA through hydrolytic/oxidative To understand the drug–protein interaction of which ultimate molecular target was DNA, the affinity of compounds towards HSA was also investigated by the docking and further validated by spectroscopic techniques and DFT calculations which showed hydrophobic interaction in the subdomain IIA of HSA. Furthermore, complexes showed high inhibitory activity against Topo-Iα at a concentration of 5-20 μM as IC50, suggesting that complexes are efficiently DNA cleaving agent. *In vitro* studies on the anticancer activity against the cell lines revealed that complexes have the capability to kill the chosen cancer cell, but the efficiency of few complexes are higher than the reported earlier. The mode of cell death induced by complex is primarily apoptosis as revealed by staining, Hoechst 33258 staining, and assessment of the mitochondrial trans-membrane potential.

IL-50

Druggable Space beyond the rule of 5

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Abstract: Despite the advances in combinatorial chemistry, high throughput and virtual screening experiments, plethora of clinical studies disquiet due to lead and drug-likeness attritions. The opportunities of chemical space beyond the rule of five were examined to improve the discovery of drugs. Known descriptive molecular property filters proposed by Lipinski, Verber and Hann are not efficient enough to encompass long array of compounds. Also, these filters do not consider the specificity of biological target. In this pursuit we have tried to appraise eight molecular properties for two major classes of biological targets viz membrane proteins and ion channels binding ligands. These molecular properties were utilized to search for the specific attributes that can be identified as an intervening space for dictating the biological activity.

IL-51

Evaluation of Antimicrobial, DNA cleavage and anticancer activities of transition metal Schiff base complexes

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Abstract: Now a days chemotherapy and radiotherapy are mostly used for various cancer treatments. The platinum metal containing cisplatin is today among the most widely used cytotoxic drug for cancer treatment. Since many cancer cells are resistant to radiotherapy and/or several chemotherapeutic drugs, the synthesis of new bio-reductive molecules might be an innovative strategy. Hence, the investigation of the anticarcinogenic potential of Schiff base derivatives gains crucial importance. Schiff bases have the capability to bind DNA and proteins, which results in the cytotoxicity of tumour cells[1-7].In this presentation we describe the transition metal complexes{(Cr(III), VO(V), Pd(II) and Pt(II) with bidentate Schiff base ligands(2-hydroxy-1-naphthalenylmethylene hydrazinecarboxamide, 2-Hydroxy-1-naphthalenylmethylene hydrazinecarbothioamide, 3-formyl-4-chlorocoumarin hydrazinecarbothioamide and 3-formyl-4-chlorocoumarin hydrazinecarboxamide). The metal complexes have been synthesized by the reaction of metal salts andSchiff base ligands. All the synthesized compounds have been characterized by elemental analyses, melting point determinations, and a combination of electronic, FT-IR, ^{1}H-NMR, ^{13}C-NMR, UV-Vis, mass and X-ray diffraction(XRD) spectroscopic studies. The newly synthesized complexes manifested significant *in vitro* cytotoxic activity against human MCF-7 breast adenocarcinoma cancer cell line.Additionally, antimicrobial effects of both the ligands and their complexes on different bacteria and fungi have been recorded and these are found to possess significant fungicidal and bactericidal properties.Further, free ligands and their complexes have been screened for their DNA cleavage activity. The details of these findings will be discussed.

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IL-52

Catalytic and Enantioselective Synthesis of Benzoxasiloles: Direct Application to (*R*)-Orphenadrine and (*S*)-Neobenodine

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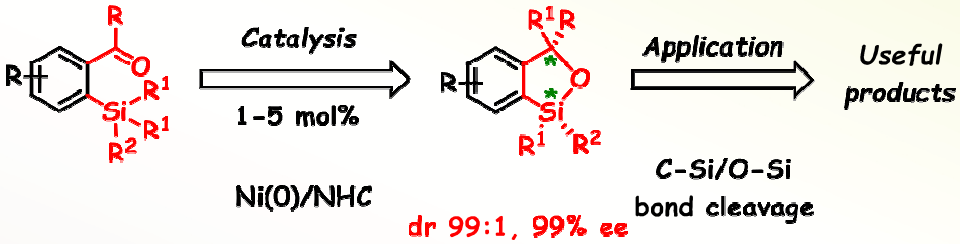
Abstract: Benzoxasiloles are building blocks of high synthetic potential for several direct transformations to useful products. Here, the development of catalytic and highly enantioselective synthesis of 3-aryl-, vinyl- and alkynyl-2,1-benzoxasiloles will be presented starting from benzaldehydes having aryl-, vinyl-, and alkynylsilyl groups at the ortho position. Nickel(0)/N-heterocyclic carbine catalyzed racemic as well as asymmetric synthesis will be discussed. Extensive mechanistic studies were carried out with the help of NMR for racemic and for chiral synthesis and an interesting switching mechanism was evolved, which will be discussed in detail.

As it has chemically reactive C-Si and O-Si bonds, was exploited for the synthesis of various useful building blocks, such as diarylmethanols and optically enriched antihistamic and anticholinergic drug molecules (R)-orphenadrine and (S)- neobenodine.

The key features of above developed method are environmental benign in nature, cheap feedstock materials, low catalyst loading (1 mol%), atom-econmic, excellent diastereo- and enantioselective (ca 99% dr and 99% ee).



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IL-53

Integrating Sustainable Chemistryin Pharmaceutical Research: Novel Transition Metal-free Approaches for Drug Discovery and Development

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Abstract: The hazardous effect of the chemical processes involved to manufacture drugs and pharmaceuticals on the environment has ushered the need for sustainable chemistry development. In compliance with the regulatory guidelines of the Environment Protection Agency the pharmaceutical industries plan to prioritise R & D targets towards the fulfilment of the 'triple bottom line' philosophy of green chemistry[1] for green and clean synthesis that include minimization of (i) waste generation, (ii) use of auxiliary substances (e.g., organic solvents, additional reagents) and (iii) use of energy. Seemingly, the sustainable development is not restricted to the domain of pharma industries and the green chemistry tools have increasing influence on medicinal chemistry and chemistry research based organisations.[2]

Managing the atom economy is the key component in the 'triple bottom line philosophy' of green chemistry to minimize waste generation and can be addressed by adopting/devising catalytic methods. However, though the use of transition-metal based catalysts is a popular choice the toxic effect of most of the transition metal salts/complexes urge for alternatives. This led to the upsurge of metal-free catalytic procedures. However, a molecular level understanding on the origin of catalysis for such metal-free processes that would promote their rational uses is highly desirable. Towards this initiative, the present discussion would focus on origin of the catalytic potential of ionic liquids,[3] fluorous alcohols,[4] and aqueous medium[5] demonstrating the applicability in the drug discovery and development.[6]

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IL-54

Nanocrystal Based Topical Formulations for the Treatment of Fungal Infections

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Abstract: The occurrence of fungal infection is on increasing edge due to change in the environmental conditions and lifestyle. Superficial fungal infections have a greater share of various skin infections; hence its management becomes the priority. Amongst different types of fungal infections, *Candida albicans*related infections are most prevailing. The major problem faced with the conventional drug regime is increasing frequency of dosing thereby increasing the risk of adverse effects and this reduces patient compliance and due to the short residence time of drug the relapse rates are high. This paves a way for development of novel drug delivery systems that have added advantages of overcoming the shortcomings of conventional therapy. Nanocrystals, being crystals of 100% pure drug, minimizes the risk of incompatibility with excipientsand has potential for targeted drug delivery owing to their narrow particle size distribution. They aid in increasing the solubility and penetration hence, may prove to be effective in improving the bioavailability. Stability of nanocrystals plays an important role in promoting its safety and efficacy of drugs. Nanocrystals have been explored and have captured the market for oral and injectable delivery systems. Many researchers have found promising results with nanocystals to be used for topical drug delivery.Nanocrystals have highest drug loading as compared to other nano-based formulations and require low quantity ofsurfactants for stabilization; thus they are safer for topical use. The presentation covers the challenges, opportunities, application and future prospects of nanocrystals in the treatment of fungal diseases.

IL-55

Meeting the neurodegenerative disease at the junction of chemical, biological and behavioral science

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Abstract: Neurodegenerative disease (ND) takes heavy tolls by ruining the quality of life in various aspects. ND can impair the cognitive function, motor activity, learning process and variousother functions. Even this social disorder is known for more than half a century, not much disease modifying treatments are available beside some palliative management. However, quite a bit advance has been made about the knowledge related to the disease progression raises the hopes for better management of the socially challenging ND. My lab is currently investigating the Alzheimer disease (AD), Parkinsonism (PD), Amyotrophic Lateral Sclerosis and other among various ND that causes cognitive decline. We are trying to develop therapeutic strategy that is mechanism based and poised to reverse or ameliorate the pathological symptoms and survival. The goal is to the understand and achieve the correlation between behavioral aspects of the disease and cognitive decline using a mechanism-based treatment module. In last decades, many clinical trials have been failed to manage ND symptomatic phenotype raises concern about the correlation study and deeper understanding to facilitate the successful translation. Our lab is dedicated to regulate and modify the toxic protein that disrupts the various cytoskeletal associated process acting as a tipping point of an array of protopathic disease such as AD, PD, a few to name. We design phyto-construct that has the ability to alter plasticity of malign protein responsible for inducing pathological symptoms over the period of time. This phyto-construct has the ability to quality control the proteotoxic protein and kinetically stabilize them to reverse their toxic gain of function. How this phyto-construct reverse protopathic phenotype such as memory deficit, cognitive function, motor movement, muscular rigidity and other behavioral traits, is a key concern of our study. Bridging a gap between molecular cause of the ND and behavioral modulation remains a key challenge to combat the series of socially challenging ND to achieve a sensible therapeutic advance and tangible benefit for patients.

IL-56

CHEMICAL AND BIOLOGICAL EXPLORATION OF INDIAN MEDICINAL PLANTSFOR HUMAN HEALTH CARE

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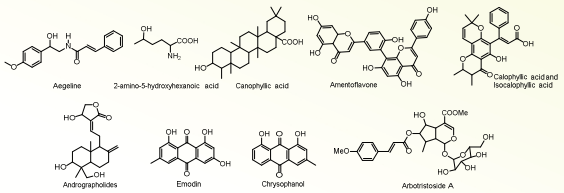
Abstract: In continuation of drug discovery program on the Indian Medicinal Plants we identified several bioactive molecules for diseases such as diabetes, dyslipidemia, cancer etc. From *Aegle marmelos*[1] we identified an alkaloidal amide (aegeline), which exhibits *invivo* antihyperglycemic activity and lipid lowering activity. A series of synthetic compounds related to aegeline have been synthesized and evaluated for their antidyslipidemic and antioxidant activity.[2,3]We isolated an unusual amino acid, i.e. 2-amino-5-hydroxyhexanoic acid from the seeds of *Crotalaria juncea*,[4]andcanophyllic acid, amentoflavone and calophyllic acid and isocalophyllic acid from the leaves of *Calophyllum inophyllum*,[5] which showed lipid lowering activity in the in vivo experiments. Andrographolide has been identified as one of the active constituents against atherosclerosis from *Andrographis paniculata*. We synthesized few novel derivatives of andrographolide to improve their antidyslipidemic, LDL-oxidation and antioxidant activity.[6]We also isolated few anticancer compounds such as anthraquinones (emodin and chrysophanol) from *Rheum emodi*[7,8] and iridoids (arbotristoside A) from *Nyctanthes arbortristis*and a large number of derivatives were synthesized and studied their activity.[9] The structure activity relationships, mechanistic aspects and improvement in their therapeutic activity will be discussed.



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IL-57

DIVERSITY ORIENTED SYNTHESIS APPROACH FOR MACROCYCLES

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ABSTRACT: In drug discovery and chemical genetics, design and synthesis of molecular libraries with diverse structures to address diverse biological functions is an important yet challenging task. (Driggers *et al.*, 2008; Schneider, 2018)Macrocycles are structurally diverse molecules that possess an organized yet flexible structure have gained significant consideration in recent times. macrocycles are excellent candidates for mechanistic and binding studies for various biological processes because of their ability to achieve optimal binding to difficult targets. (Marsault and Peterson, 2011; Giordanetto and Kihlberg, 2014) The most suitable and well-established strategy divulged for the construction of such diverse macrocycles is diversity-oriented synthesis (DOS) approach utilizing build/couple/pair (B/C/P) synthetic algorithms. (Burke and Schreiber, 2004; Grossmann *et al.*, 2014; Nie *et al.*, 2016; Maurya and Rana, 2017; Rana *et al.*, 2018) Herein, we outlined an application of new Build/Couple/Pair synthetic sequencetowards the synthesis of a library of macrocycles.

KEYWORDS: Amino acids; diversity-oriented synthesis; macrocycles; drug discovery;ciprofloxacin

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IL-58

Unique Rearrangements of β-Aryloxyacrylates and δ-Hydroxy-alkynones Under Mild Acid Catalysis

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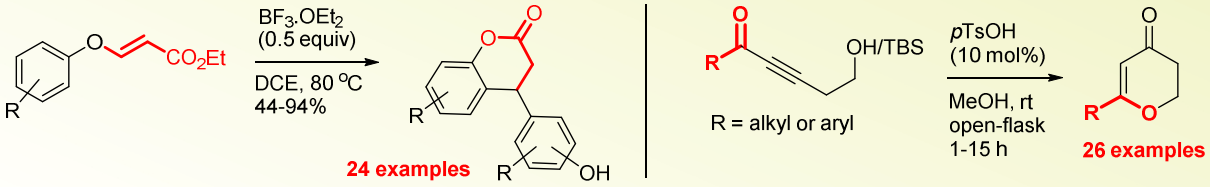
Abstract: Unique rearrangements of β-aryloxyacrylatescatalyzed by the Lewis acid $BF_3.OEt_2$ to 4-aryldihydrocoumarins has been developed.[1] 4-Aryldihydrocoumarins are important natural products and are evaluated for various biological activities.[2] Also a benign *p*-TsOHcatalyzed rearrangement of δ-hydroxy-alkynones to 2,3-dihydropyran-4-ones has been investigated. Dihydropyranone based natural products have varied bioactivities. This chemistry has been utilized in the synthesis of natural products.[3] The lecture will give the insights of these two new rearrangements.



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IL-59

Beneficial effects of Bergenin in Alzheimer's disease: In silico, in vitro and invivo evaluation

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Abstract: Bergenin is known for antioxidant, antiulcerogenic, hepatoprotective, neuroprotective, anti-inflammatory and wound healing properties. It has been reported to have β-secretase (BACE-1) enzyme inhibitory activity and prevented neuronal death in the primary culture of rat cortical neurons. In present study Bergenin was screened by molecular docking using GOLD suite (version 5.2), CCDC for predicting its activity against targets of AD management like acetylcholinesterase (AChE) (1B41), butyrylcholinesterase (BuChE) (1P0I), Tau protein kinase 1 (GSK-3β) (1J1B), BACE-1 (1FKN) wherein the GOLD score and fitness of bergenin were comparable to those of standard drugs like donepezil, galanthamine, physostigmine, etc. Bergenin also showed dose-dependent inhibition of cholinesterases and found to be safe up to 50 µM on SH-SY5Y cell lines in cytotoxicity studies. It was evaluated at three dose levels (20, 40 and 80 mg/kg; p.o.) in scopolamine induced amnesia (2 mg/kg, i.p.) and also in streptozotocin (3 mg/kg, ICV, unilateral) induced AD model in Wistar rats followed by behavioural analysis by in Morris water maze and Y maze tasks. Bergenin significantly ($p < 0.01$) and dose-dependently alleviated amnesia induced by scopolamine and could significantly ameliorate STZ induced behavioral deficits, inhibit the AChE and BuChE activity in parallel with an increase in the diminished GSH levels at the higher doses. The observed effects might be attributed to the cholinesterase inhibitory activity, antioxidant activity, and effects on pathological hallmarks of AD like of $A\beta_{-1-42}$ and p-tau levels which were found reduced up on supplementation of bergenin.

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IL-60

Model Informed Precision Dosing for Pediatric Population

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Abstract: Model informed precision dosing is a next generation dosing paradigm, in which drug dose is predicted based on characteristics of an individual (e.g., age, body size, organ function, genetics of drug receptors and enzymes and transporters, drug interactions, etc.) with a purpose to improve efficacy and/or lower toxicity, unlike traditional dosing, which is based on 'one-fits-all' concept. The presentation will discuss the recent foray in this direction in speakers' laboratories for predicting dosing for acetaminophen in pediatric population of different age groups.

IL-61

Human space medicine: stability issues with case studies and countermeasures

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Abstract: Stability of pharmaceuticals is of paramount importance to ensure health and wellness of astronauts on space exploration missions. On Earth, sunlight (UV-visible radiation) is one of the major factor affecting their stability. It is mandatory to evaluate the photostability of medicines as per ICH Q1B guideline "Photostability Testing of New Drug Substances and Products". But, the spacecraft radiation environment is different and complicated than terrestrial radiation environment. The penetrating space radiations and secondary radiations can alter physical and chemical stability of the medicines flown to spacecraft, which has also been reported in the published literature. Therefore, ICH 1B guideline may not suffice to predict stability of medicines during space missions.

Stability studies in simulated space radiation environment of four drugs will be presented and degradation profile will be compared with photo degradation study. All the drugs and its impurities were estimated using HPLC method. Countermeasures like choice of packaging material, formulation strategies will be discussed in session.

IL-62

Isocyanide Insertion Reactions: Our Findings

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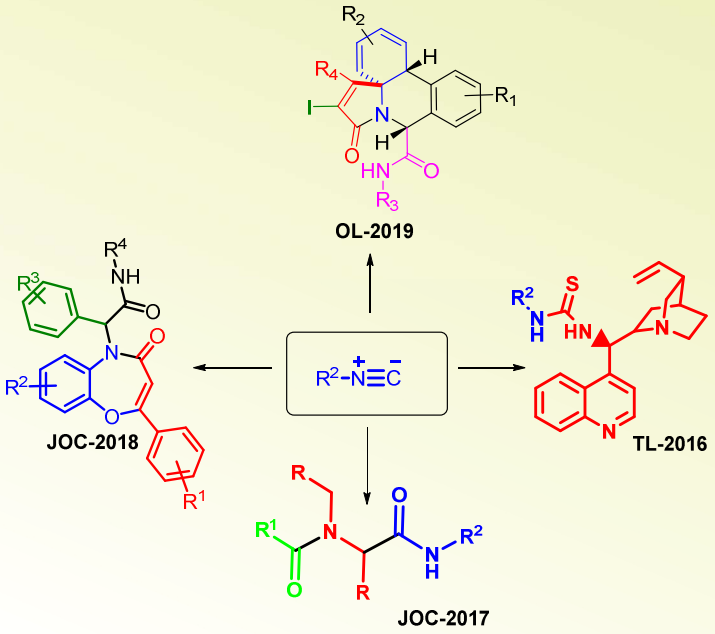

Abstract: Isocyanides have a long history in organic chemistry and have been used from academia to industryIt is one of the most versatile and extensively examined stable divalent carbon nucleophile having interesting ability of forming multiple bonds on the terminal carbon. It has drawn enduring attention because of ubiquitous application in organometallics where isocyanides are a well-studied family of ligands and in combinatorial syntheses where new desired products could be found by the isocyanide based multi-component processes such as Passirini and Ugi reactions. Herein, we will show our recent contribution to the isocyanide chemistry for the synthesis of many medicinally important sccafolds.[1-4]

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IL-63

Involvement of PTEN expression in antitumour activity of febuxostat against 4-Nitro quinolone induced oral cancer in rats

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Abstract:

Background: Breast cancer is the second most common cause of death among women worldwide after lung cancer. It occurs when certain cells in the breast become abnormal and multiply uncontrollably to form a tumour. This event occurs due to various genetic and environmental factors. These factors are responsible for activating various pathways including Ras/raf, PI3k/Akt and Wnt pathways. Febuxostat, a non-purine xanthine oxidase inhibitor is prescribed for the treatment of gout. No evidence is available for the pharmacological action of Febuxostat in breast cancer.

Objective: The objective of the present study was toinvestigate the pharmacological action and mechanism of action of febuxostat in 7, 12-dimethyl benz[a]anthracene induced breast cancer in female Wistar rats.

Materials and methods: The induction of breast cancer was done by subcutaneous injection of 7, 12-dimethyl benz[a]anthracene (45mg/kg) in the mammary gland of female Wistar rats. The animals were divided into nine different groups as per the treatment regimen. Doxorubicin was used as a standard treatment (4 mg/kg) whereas febuxostat (4.11 mg/kg) was used as investigational drug. The induction of cancer was done for a period of 12 weeks followed by the treatment with either standard or investigational drugs for a period of 6 weeks. After the completion of treatment, the animals were euthanized using thiopental sodium and the tumours were collected. Various parameters related to tumour, oxidative stress parameters, inflammatory markers and the genetic expression for PTEN were evaluated together with histopathological examination. Apart from these, histological evaluations were also done by haematoxylene-eosin staining.

Results: There was significant improvement in tumour related parameters, antioxidant parameters and anti-inflammatory markers in febuxostat treated animals as compared to the disease control animals. decrease in tumour volume and tumour burden in doxorubicin treated animals ($p<0.001$) as compared to the disease control animals. Further, there was significant decrease in tumour volume and tumour burden in febuxostat ($p<0.001$) treated animals. The survival rate and tumour inhibition ratewere also increased in treated animals as compared to the disease control groups. Further there was no expression of PTEN gene in disease control group whereas the expression was higher in doxorubicin treated animals and moderate in febuxostat treated animals.

Conclusion: From the above results it can be depicted that febuxostat exerted protective effects in DMBA induced breast cancer model in rats. This might be due to the antioxidant property and inhibitory effect on inflammatory markers like IL-6, IL-1β and TNF-α together with moderate expression of PTEN in febuxostat.

ORAL

O-1

Asymmetric syntheses identify preferred stereochemistry in small molecule allosteric modulators of the neuropeptide Y4 receptor

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Abstract: The neuropeptide Y4 receptor (Y4) is a GPCRbelonging to a family of five receptors that bind ligands neuropeptide Y (NPY), peptide YY (PYY), and pancreatic polypeptide (PP). These ligands are hormones that play important roles in the regulation of feeding behavior and energy homeostasis.Small molecule ligands that selectively activate the Y4 receptor are potential therapeutics for obesity. Currently, there is a lack of non-peptide Y4-selective ligands available for studying Y4. Having recently identified multiple small molecule Y4 ligands via HTS, optimization of these hits is ongoing. The objective of the work described here is to develop asymmetric syntheses of two confirmed small molecule Y4 ligands, enabling determination of the preferred stereochemistry for Y4 activity and facilitatingfurther optimization efforts.

Four diastereomers of Y4 PAM tBPC were synthesized to > 87% d.e.and two enantiomers of Y4 NAM VU0637120 were synthesized to >99% e.e. by employing commercially available chiral starting materials. (*S*)-VU0637120 was highly preferred for Y4 activity compared to (*R*)-VU0637120. A library based on (*S*)-VU0637120 was subsequently synthesized and obtained results enable the further optimization of these compounds in the context of the preferred stereochemistry, enhancing the probability of identifying optimized tools for studying the Y4 receptor.

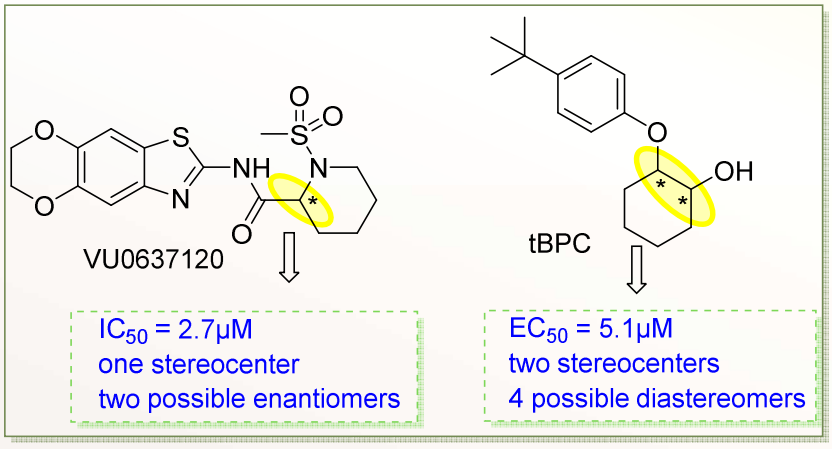

Figure 1: Structure of Y4 hits tBPC and VU0637120

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O-2

Strategies for Antileishmanial Drug Development: *De novo* Drug Discovery and Drug Repurposing

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Abstract: Visceral leishmaniasis (VL) or Kala-azar, an immuno-suppressive protozoan disease caused by *Leishmania spp.*, is being treated with the drugs which have resistance issue and serious adverse effects at their effective doses.Thus, speedy discovery of new therapeutic options is the need of the hour. *De novo* drug discovery (development of new chemical entity) and drug repurposing (new uses of old drugs) are the two available tactics for the development of new therapies against a vast number of infectious diseases. Following *De novo* drug discovery approach, we have identified three novel leads with chalcone, quinazolinone and nitroimidazole backbones having very promising *in vitro* and *in vivo* antileishmanial potential. These derivatives showed 84.48 (at 100 mg/kg × 5 days, oral dose), 80.93 (at 50 mg/kg × 5 days, intraperitoneal dose) and 99.90% (at 50 mg/kg × 5 days, oral dose) efficacy, respectively in animal model of VL. The efficacy data with the support of other studies (apoptosis studies, cytokines response and nitric oxide assay) suggested that these molecules are prospective pre-clinical candidates for the treatment of VL. Next, we exploited drug repurposing approach and selected two well-known immunomodulators, Lentinan (anti-tumor effect) and Leptin (immunoregulatory action) and evaluated their antileishmanial efficacy and effect on host's immune responses when giveneither alone or in combination with a lower dose of standard drug, miltefosine against active VL infection in mouse model.Our results demonstrated that animals that received Leptin+Miltefosine or Lentinan+Miltefosine therapy showed sterile cure (~100% inhibition of parasites) in both liver and spleen and displayed significantly increased level of host-protective cytokines (IFN-γ, IL-12 and TNF-α) along with nitric oxide. Furthermore, suppressed level of parasite-protective cytokines (IL-10, IL-4 and TGF-β), enhanced IgG2 level, splenocyte proliferation and induced phagocytic ability of macrophages during combination therapy also supported that these adjunct therapies may be exploited further for detailed investigations at pre-clinical stage for VL treatment.

O-3

In-silico target identification of novel anti-leishmanial β-carboline analogues

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Abstract: A neglected tropical disease which is a vector born, caused by flagellated protozoans of the genus *Leishmania,* communicated by the bite of female *Phlebotomine* sandfly is known as Leishmania. Presently, 1 Billion people are at risk, around 50,000 to 90,000 new cases were listed with Visceral leishmaniasis, and 20,000 to 30,000 deaths occur annually. Around90% of the new cases occur in seven countries, and50% of patients are under 15 years old, mostly in India, Brazil, and Sudan[1].Leishmaniasis control is majorly dependent upon chemotherapy that includes decade-olddrugs due to nonavailability of effective vaccines[2]. In the present *in-silico* study, titled novel β-carboline derivatives were docked against various targets of Leishmania[3] which include: Trypanothione reductase (PDB-2JK6, 1BZL), Nitric oxide synthase (PDB-1TLL,1F20), Spermidine synthase (PDB-2HTE, 6QMM)[4] and studied the interactions by comparing with the co-crystallized ligand. Pharmacokinetic studies like Absorption, Distribution, Metabolism, Excretion (ADME) was also predicted to check the druggability of the designed ligands.The results of the study revealed that the designed ligands were obeyed the rule (Lipinski rule). The output of the docking study discloses, Glide scores of the designed ligands were lied in between -11.00 to -7.52 kcal/mol and the co-crystallized ligand -19.57 to -8.46 kcal/mol in various targets. Intensely studying the amino acid residues which involved in the distinctbond formation (Hydrogen bond, Aromatic bond, Pi-Pi interactions, Halogen bonds) of the active site of the targeted PDBs with the designed ligands and cocrystal ligand, We may propose trypanothione reductase may be the probable target for the titled β-carboline analogs.

Keywords: Leishmaniasis, β-carboline, Docking studies

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O-4

Versatile Arene-Ruthenium(II)-Phosphine Complexes: From Green Catalysts for Hydration of Nitriles to Anticancer Agents

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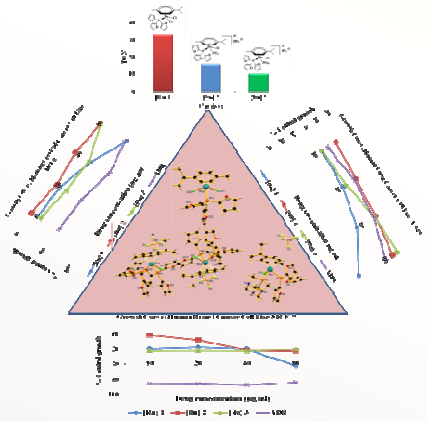
Abstract: Three new arene-ruthenium(II) complexes were prepared by treating [{RuCl(μ-Cl)(η^6-arene)}$_2$] (η^6-arene=*p*-cymene) dimer with tri(2-furyl)phosphine (PFu_3) and 1,3,5-triaza-7-phosphaadamantane (PTA), respectively, which furnished complexes viz. [$RuCl_2$(η^6-arene)PFu_3] **[Ru]-1**, [RuCl(η^6-arene)(PFu_3)(PTA)]BF_4 **[Ru]-2** and [RuCl(η^6-arene)(PFu_3)$_2$]BF_4**[Ru]-3**. All the complexes were structurally identified using different analytical methods including single-crystal X-ray crystallography. The effectiveness of resulting complexes as probable homogeneous catalysts for hydration of different nitriles in selective manner into corresponding amides in aqueous medium and aerial atmosphere was explored. There was a remarkable variation in efficiencies of the catalysts based on the nature and number of phosphorous-donor ligands and sites available for catalysis. Experimental studies performed using structural analogues of different catalysts concluded a structural-activity relationship for the relatively higher activity of **[Ru]-1**, which is efficient to convert number of aromatic, heteroaromatic and aliphatic nitriles. The use of eco-friendly water as a solvent, open atmosphere and avoidance of any organic solvent during the catalytic reactions prove the reported process to be truly green and sustainable. The anticancer activity of the reported complexes has been tested against three different cancer cell lines viz., breast cancer cell line MCF7, lung cancer cell line A549 and cervix cancer cell line HeLa. All the complexes have shown promising antiproliferative activity comparable to Adriamycin.

Keywords: Green Chemistry, Homogeneous Catalysis, Ru(II)-Arene Complexes, Anti-proliferative activity



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O-5

EVALUATION OF *EUPHORIA LONGANA* IN ORAL CANCER INDUCED RATS ASSOCIATED WITH TYPE II DIABETES MELLITUS

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Abstract: Oral cancer has been the sixth most common occurring subtype of head and neck cancer worldwide. For the progression of oral cancer, diabetes mellitus type II becomes a risk factor due to the oxidative is a risk factor for development of oral cancer which might be due to the enhanced oxidative stress in diabetic condition that leads to the progression of cancer.DimocarpusLongan (*Euphoria longana*) is a fruit of subtropical climate that belongs to the lychee family, Sapindaceae. High amount of polyphenolssuch as gallic acid, corilagin and ellagic acid is found in the seeds of longanaas compared to the fruit.The treatment with *Euphoria longana*showed protective effect in4-NQO induced oral cancer and the combination of *Euphoria longana*with other chemotherapeutic agent might be beneficial to improve the diseased condition than using a chemotherapeutic agent alone. Also in the animals induced with diabetes as well as oral cancer, the combined treatment has reduced the progression of disease as compared to the treatment given alone. Hence this might prove to contribute for beneficial and therapeutic approach in the treatment of oral cancer associated with diabetes mellitus type II.

O-6

DIVERSE STRATEGIES TO BOOST UP SOLUBILITY OF POOR WATER SOLUBLE DRUGS - A REVIEW

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ABSTRACT: As we understand that for achieving a supportive effect in the human body, the prescription should be bioavailable and in this way it depends upon the dissolvability of the drug. Starting late 40% of the meds are inadequate water dissolvable which produces responses, for instance, gastric exacerbation, peptic ulceration, etc. While just 8% of new medication up-and-comers have both high dissolvability and penetrability. For BCS class II drugs, redesign of dissolvability is a huge parameter before the arrangement of estimations structure. The purpose of this review is to improve the solubilization and bioavailability of insufficiently dissolvable sedates by using various approaches like physical, invention and others changes or systems and included BCS course of action, transporters for dissolvability. Update and different techniques for dissolvability improvement.

KEYWORDS: Solubility, Bioavailability, Solubility improvement techniques, Poorly water-soluble medicine.

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O-7

Transformation of Different Sulfides to its Sulfoxide by a Plant Peroxidase

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ABSTRACT: Chiral organic sulfoxides are important synthons and chiral auxiliaries in synthetic organic chemistry. Therefore, synthesis of chiral sulfoxide is an active area of continuing research interest. The most common method for the preparation of sulfoxide is by the oxidation of their corresponding sulfides. Both the chemical and biological catalysts have been developed for this purpose. Though, the reaction conditions for the preparation of chiral organic sulfoxides. With hope that some of them will produce the desired sulfoxides in a good enantiomeric excess.

An enzyme from a new source has been purified to homogeneity using a simple procedure involving concentration by ultra filtration and anion exchange chromatography on diethyl amino ethyl [DEAE] cellulose column. Sodium dodecyl sulphate-polyacrylamide gel electrophoresis [SDS PAGE] analysis of the purified enzyme has shown a single protein band of molecular mass 43.0 k Da which has been confirmed by NATIVE-PAGE. The pH and temperature optima of the enzyme were 3.0 and 298 K, respectively. The enzyme transformed approximately 97% methyl phenyl sulfide to its sulfoxide. The product was racemic mixture. The source of the enzyme is conveniently available and the enzyme could be purified using a simpler procedure.

Keywords: Plant enzyme , Sulfoxide, Musa paradisiaca, Metalloenzyme.

O-8

Synthesis and *in vitro* pharmacological characterization of pyrimidinium ionic liquids

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Abstract: A library of *N*-alkyl, *N*-arylalkyl, and *N*-aryloxy alkyl pyrimidinium ionic liquids coupled with tetrafluoroborate and bis(trifluoromethane)sulfonamide (BF_4 and NTf_2) as counter anions were prepared synthetically in two steps with overall isolated yields. Their physicochemical and chemical structures were determined using different analysis techniques: NMR, mass, FTIR, CHNS elemental analyzers, UV, DSC, and TGA. The pharmacological characterization of the synthesized ionic liquids has been evaluated by investigating their *in vitro* minimum inhibitory concentration (MIC) study against several pathogenic microbes (bacteria and fungi) and amongst all of the compounds *N*-alkyl substituted ionic liquids:$[C_9Pym]BF_4$ and $[C_{10}Pym]BF_4$ containing longer alkyl chain length and *N*-arylalkyl and *N*-aryloxy alkyl substituted ionic liquids:$[(PhC_2)Pym]BF_4$, $[(PhC_3)Pym]BF_4$), $[(PhOC_3)Pym]BF_4$) and $[(PhOC_4)Pym]BF_4$) exhibit moderate to good bioactivity [1-2]. Further, our efforts have also been engaged towards finding anticancer effect (Cytotoxicity assay) against a panel of four human cancer cell lines: Caco-2, AGS cell, lung cancer A549 cell and breast cancer T47 D cell lines using MTT, and Trypan Blue assay. It can be concluded that among all of the compounds $[C_9Pyr]BF_4$ and $[C_{10}Pyr]BF_4$ containing longer alkyl chain was found to significantly inhibit the growth of studied cell lines in a dose-dependent manner with IC_{50} values at 50 μM after 24 h of treatment. According to the structure-activity relationships (SAR) study, the chain length of alkyl substitution on the cation with different anions could play an important role in the cytotoxicity of these ionic liquids. Therefore, these results show a very promising future for the application of the ionic liquids based on pyrimidine as possible antimicrobial and anticancer agents in microbial, and cancer treatment.

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O-9

Highly sustainable approach towards synthesis of pharmaceutically relevant molecules

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Abstract: Synthesis of drugs that is being carried out currently is not quite sustainable. In fact, current environmental policies require synthetic chemist to divert or design a more sustainable process for such synthesis. In this scenario, where water is mainly considered as an enemy of organic chemist, at least this is how organic chemistry is taught in academic settings could be a good option. There are few or no processes to synthesize organic molecules in using water as solvent described in undergraduate course. This is partly true due to handling of water sensitive reagents in hydrous conditionsis a big challenge. Although, there are many reactions which are done in such dry conditions but could also be performed in water with same or higher efficiency. If not anhydrous, a solubility issues always come forward when water alone is used as a solvent for highly lipophilic substrates. Our research mainly focuses towards solving these challenges using water and small amount of biodegradable surfactant as a solvent system[1, 2]. Now, with such system, and tailormade lipophilic catalysts/ligands, we can now efficiently synthesize pharmaceutically relevant molecules in an environmentally responsible manner. Following representative molecules weresynthesized in water using only *few hundreds ppm of endangered costly metal* (palladium) catalyst (Figure 1).[2]

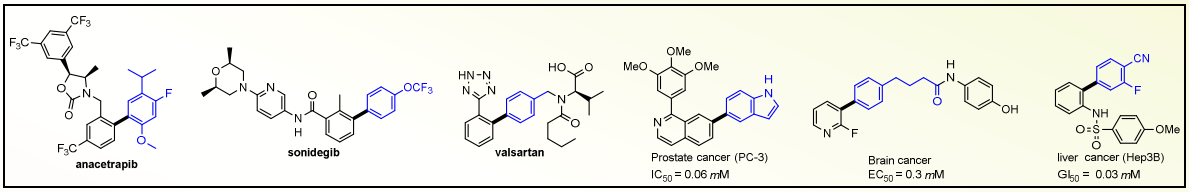

Figure 1. Synthesis of drug intermediates using 300-500 ppm of Pd

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O-10

Synthesis of Therapeutic significant oxadiazole analogs and its crystallographic studies.

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Abstract: A series of isoxazole-oxadiazole hybrid analogs was designed and synthesized with the aim to target several viruses including picornavirus. Recent publication shows that the isoxazole-oxadiazole scaffold is a promising $S1P_1$ receptor agonist[1,2,3]and it plays a fundamental physiological role in vascular development and stabilization, lymphocyte migration, and proliferation. However, oxadiazole synthesis has been explored extensively to access the medicinal values of the molecules.

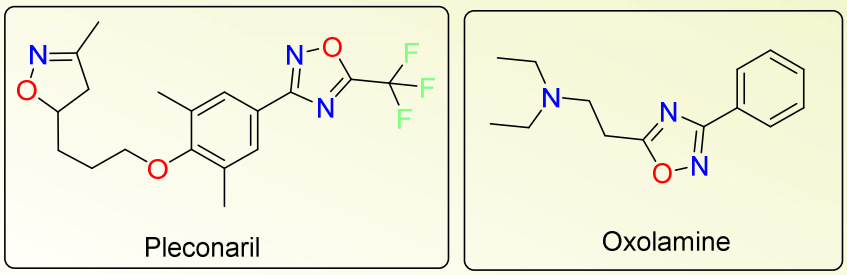

Figure 1: Clinically important molecule containing isoxazole-oxadiazole moiety.

Herein we report the novel synthetic method to prepare isoxazole-oxadiazole hybrid scaffold. The key intermediate was synthesized by hydroxylamine hydrochloride and further it was cyclized in oxadiazole by treating it with amide coupling reagent followed by refluxed in ethanol.

Acknowledgment: Authors acknowledge to DST-SERB (EMR/2017/003331) for our financial support.

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O-11

Studies on Moringa based flocculant for the treatment of wastewater

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Abstract: Natural polymer and its modified derivatives have been extensively used in many applications. Moringa gum was found to contain L-arabinose, D-galactose, D-glucuronic acid, L-rhamnose, D-mannose, and D-xylose in the molar ratios of 14.5:11.3:3:2:1:1. In the present study, the purified Moringa gum exudate from the drum stick plant was modified by graft copolymerization reaction using a microwave-assisted method. The reaction was carried out by using acrylamide(PAM) as a monomer and ceric ammonium nitrate(CAN) as initiator. The synthesized graft copolymer was characterized by FTIR, TGA, DSC, FE-SEM and used as flocculant for wastewater treatment. Grafted material shows greater intrinsic viscosity property which proves that material was best for the used as flocculant. The flocculation characteristics of grafted and ungrafted polysaccharides were evaluated in Kaolin suspension, Coal fine, and wastewater.

Keywords: Moringa gum, polyacrylamide, microwave-assisted synthesis, graft copolymer, wastewater treatment.

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O-12

Synthesized and computational prediction of furfuraldehyde-sulfonamide Schiff base compounds and their antibacterial activity

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Abstract: The development of new antibacterial hybrid molecules which could remain more effective against invasive microorganism and resistant to bacterial strains and also significantly inhibited the growth of microbes. A series offurfuraldehyde-sulfur conjugate Schiff base compounds (F1-F7) were synthesized by N-heteroaryl substituted sulphonamide with furfuraldehyde in glacial acetic acid. All the of synthesized compounds were structurally interpreted by FT/IR, ^{1}H NMR, and UV-visible spectroscopy technique. The preliminary *in-vitro* antimicrobial activity of all the synthesized molecules was investigated by agar well diffusion method. The molecular docking and Lipinski's rule (RO5) of all the compounds were performed. The results indicate that the compound **F4**4-((furan-2-ylmethylene) amino)-N-(5-methylisoxazol-3-yl) benzene sulfonamide was more significant inhibition against both bacterial strains whereas the compound **F3**4-((furan-2-ylmethylene) amino)-N-(pyrimidin-2-yl) benzene sulfonamide was more effective and potent antibacterial action against *E. coli*and others are moderate inhibition. These compounds were showed antibacterial actions due to presence of Furan ring and azomethine and sulfomoyl substituent in their structural frame.

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O-13

Metal-Organic Frameworks as New General Catalyst for Electrochemical Water Splitting

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Abstract: Due to depletion of fossil fuel reserves and the enhanced risk of global warming, the search for cleaner and renewable energy sources has become very important in recent years. Among several, electrochemical water splitting represent one of the most facile environment friendly energy source.[1] Because it produces oxygen and hydrogen which upon recombination will produce water to give rise to energy. Water splitting consists of two half-cell reactions; oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). Though theoretically these processes need total 1.23 V potential but the actual potential is much higher due to slow kinetics and diffusion. As result efficient catalysts are required to catalyze this reaction at a lower overpotential.

Nowadays metal-organic frameworks(MOFs) are emerging as new generation catalyst for electrochemical water splitting reaction due to permanent porosity, presence of well-defined functionalized sites etc.[2] We have synthesized a series of MOFs to catalyze the electrochemical water splitting. Depending on nature of the metal ion they catalyze OER or HER reaction with significantly low overpotential. We have also shown the effect of particle size on catalytic activity. Interestingly these MOFs shows extremely high stability under electrochemical environment.

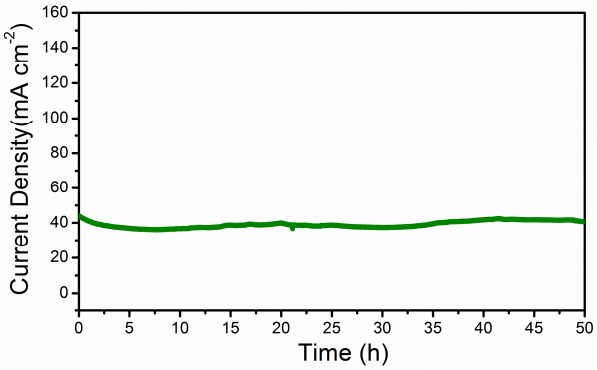

Figure 1: Chronoamperometry Studies of the MOFs catalysts showing the stability.

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O-14

Conformational influences of Phosphorylation and O-GlcNAcylation on Proline-rich domain of Tau

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Abstract: Microtubule associated protein tau (MAPT) is a phospho-protein within neurons of the brain.Weingarten et al. [1]Aggregation of tau is the leading cause of taupathies such as Alzheimer's disease. Tau undergoes several post-translational modifications of which phosphorylation and O-linked glycosylation are key chemical modifications. Tau aggregates into paired helical filaments and neuro-fibrillary tangles upon hyperphosphorylation whereas O-GlcNAcylation stabilizes the soluble form of tau. Schwalbe et al. [2] However how specific phosphorylation and/or O-GlcNAcylation events influence tau conformation remains largely unknown due to its high flexibility given the fact that phosphorylation and O-GlcNAcylation commonly occur in natively disordered regions of proteins and often have opposing functional effects. We investigated the phosphorylation and O-GlcNAcylation induced conformational effects on a tau segment from proline rich domain (P2) tau225-246, by performing metadynamics simulations employing two modern all-atom force field with different phosphorylation (pT231 and pS235 or pT231, pS235, pS237 and pS238) and O-GlcNAcylation (T231 and S235) pattern. We find that phosphorylation disrupt the nascent β-sheet pattern (^{225}KVAVVR^{230} and ^{240}KSRLQT^{245}) as a result of salt-bridge formation which is also responsible for inducing transient α-helix (^{238}SAKSRLQ^{244}) when phosphorylated at four sites. In contrast O-GlcNAcylation showed only modest effect which resembles native form of peptide. The data here suggest the opposing structural effects of both PTMs on natively disordered protein.

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O-15

ENTHALPY-ENTROPY COMPENSATION (EEC) EFFECT IN REDOX KINETICS BETWEEN PARA-SUBSTITUTED ANILINE AND PEROXOMONOSULFATE IN ACIDIC MEDIUM

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Abstract: Peroxoacids are potential oxidizing agents of considerable significance. Peroxomonosulfate is a hydrolytic product of peroxodisulfate and it is considered to be much better oxidant than its parent analogue. we are also engaged with studies of kinetics of peroxomonosulfate oxidations[1-7] Peroxomonosulfate oxidation of some para-substituted aniline in aqueous perchloric medium has been studied and leads to the formation of azoxybenzene-4-4'-disulfonic acid from Sulfanilic Acid[8]. The reaction was under second order conditions. The reaction is retarded by hydrogen ions. Various thermodynamics parameters have been reported in this study to investigate the nature of the reaction mechanism in solutions. Therefore, Isokinetic relationship and exner's equation are useful to arrive at a decision whether or not a common mechanism is operative for a series of reactions. Also, the Isokinetic parameter β is further useful in deciding whether or not the system is enthalpy controlled or entropy controlled.

Keywords: Compensation, Enthalpy, Entropy, Isokinetic Temperature, Oxidation.

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O-16

Design and Syntheses of Palladium Complexes of NNN/CNN Pincer Ligands for Catalytic Dehydrogenative Cross-Coupling of Heteroarenes

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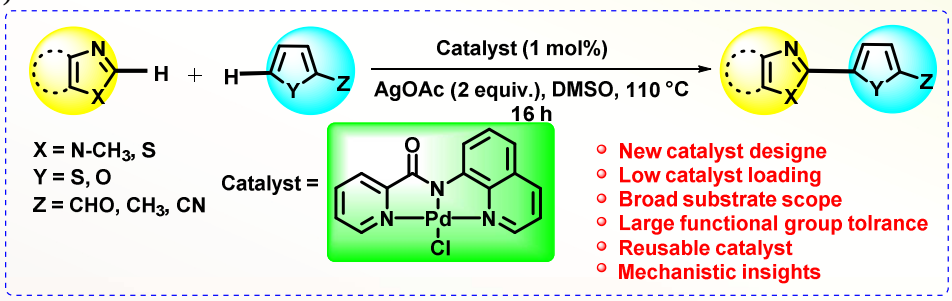
Abstract: Organopalladium compounds are one of the most versatile organometallic reagents used in organic synthesis.[1] These compounds have found widespread use as catalysts in organic synthesis for carbon-carbon and carbon-heteroatom bond formation in last four decades. Palladium catalysts offer attractive synthetic properties such as broad synthetic extent combined with prospect of controlled and selective transformations.[2]This balance is achieved by introducing efficient changes in ligand and metal center, allowing improvement in stability, reaction selectivity, complex reactivity, and fundamental catalyst design. Moreover, structural and electronic features of the metal used in catalysis can be refined by suitable choice of the chelating arms of the pincer ligand.[3]
Development of straightforward routes to construct biheteroaryl structural moieties which are usually found in several pharmaceuticals, natural products, and functional materials is of immense importance in organic synthesis.[4] The synthesis of bi-heteroarenes *via* conventional transition-metal catalyzed cross-coupling reactions requires preactivated substrate and involves several synthetic steps.[5] From the viewpoint of step economy and high efficiency, direct oxidative C-H/C-H cross-coupling of two heteroarenes would be most ideal, concise and sustainable strategy towards the synthesis of biheteroaryl compounds *via* dual C-H functionalization.[6]Due to the importance of biheteroarenes and our ongoing interest, here we report a one-pot syntheses of air stable pincer complexes and their catalytic efficiency towards cross dehydrogenative coupling reaction of heteroarenes in open air (**Scheme 1**).



Scheme 1: Synthesis of biaryl/heterobiaryl compounds

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O-17

Ruthenium Catalyzed C-H Acylmethylation of *N*-Arylphthalazine-1,4-diones with *α*-Carbonyl SulfoxoniumYlides: Highway to Diversely functionalized Phthalazino-fused Cinnolines

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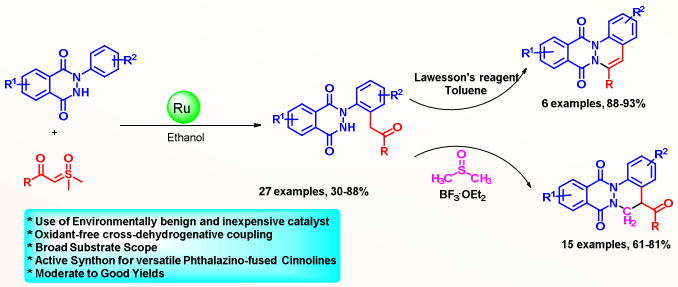
Abstract: Transition-metal-catalyzed C-C and C-N bond forming strategies have completely astonished the scientific community by endowing complex chemical entities from simple starting materials.[1]In particular, Ru-catalyzed C-H functionalization strategies have clearly marked a distinct recognition in tailoring unprecedented heterocyclic architectures.[2] In this regard, transition-metal-catalyzed annulation of 2-arylphthalazine-1,4-diones with different coupling partners, including internal alkynes, propargyl alcohols and *α*-diazo carbonyl compounds*via* C−H activation approach have attracted great interest in recent years.[3a-c]

In striking contrast to *α*-diazo carbonyl compounds, sulfoxoniumylides are convenient and safer carbene precursors that have been utilized for *o*-acylmethylationand annulationof different aromatic scaffolds, mainly through Rh/Ir/Ru catalysis.[4]Very recently, we have reported[5]a Ru(II)-catalyzed strategy for the *ortho*-Csp^2-H acylmethylation of 2-aryl-2,3-dihydrophthalazine-1,4-diones with *α*-carbonyl sulfoxoniumylides that proceeded through C-H activation, carbene generation and C-H insertion process. The synthesized 2-(*o*-acylmethylaryl)-2,3-dihydrophthalazine-1,4-diones further underwent cyclization usingLawesson's reagent in refluxing toluene under ambient conditions to afford 6-arylphthalazino[2,3-*a*]cinnoline-8,13-dione in excellent yields. While 5-acyl-5,6-dihydrophthalazino[2,3-*a*]cinnoline-8,13-diones were obtained by $BF_3{\cdot}OEt_2$-mediated cyclization of 2-(*o*-acylmethylaryl)-2,3-dihydrophthalazine-1,4-diones using DMSO as a solvent and a methylene source *via* dual C-C and C-N bond formations.Notably, the disclosed strategies showed good functional group tolerance and high atom-efficiency.



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O-18

Agreen synthesis of multifunctional thieno(3,2-*c*)pyran-4-ones from 2-pyranones

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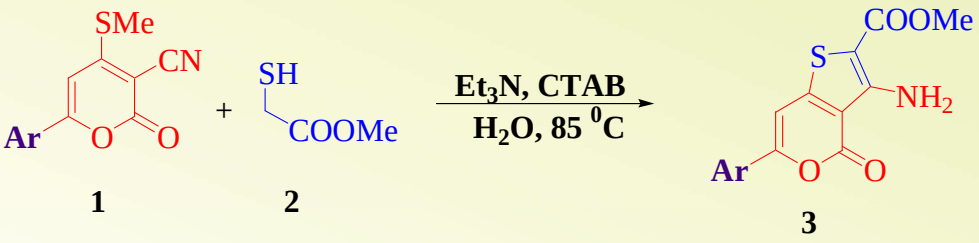

1 **2** **3**

Ar=C_6H_5, p-CH_3.C_6H_4, p-F.C_6H_4, p-Cl.C_6H_4, p-Br.C_6H_4, o-p-Cl.C_6H_3, 1-Naphthyl, 2-Naphthyl, p-OMe.C_6H_4, o-OMe.C_6H_4

Abstract: Thieno(3,2-c)pyran was synthesized and reported as antileishmanial and antifungal[1,2] but their other medicinal properties need to be established. In this connection anticancerproperties need to be evaluated as various similar heterocycles was found to be effective for cancer prevention and therapeutics [3].Recently, synthesis of indolo(2,3-*c*)pyran-1-one and thieno[2,3-c]pyrane-7-ones was reported as anticancer agents[4].Therefore we became interested to develop a new synthetic approach for thieno[3,2-*c*]pyran-4-one.One pot synthesis of thieno[3,2-*c*]pyran-4-one (**3**) was carried out in water by reaction of methylthioglycolate (**2**) and 6-aryl-4-(methylthio)-2-oxo-2*H*-pyran-3-carbonitriles (**1**) in presence oftriethylamine,CTABas surfactant. The desired product was afforded in excellent yield (80-95%). We have developed an eco-friendly, simple and water mediate methodology for the synthesis of thieno[3,2-c]pyrans. The required precursors was synthesized by reaction of methyl-2-cyano-3,3-bis(methylthio)acrylate and various acetophenones in presence of potassium hydroxide in DMSO.

Key Words: Thiophenes, Pyranothiophenes, Pyridinones, Thieno[3,2-*c*]pyran-4-one.

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O-19

3D-QSAR and Ligand Based Pharmacophore Modelling of Poly ADP-Ribose Polymerase 1 (PARP1) Inhibitors

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Abstract: Poly ADP-Ribose Polymerase 1 (PARP1) is one of the potential target for treatment of cancer, specifically for BRCAm breast and ovarian cancer. There are currently four FDA approved PARP1 inhibitors namely Olaparib, Rucaparib,Niraparib and Tolazoparibin the market. All these PARP1 inhibitors are non-selective NAD^+ analogues which also cause concurrent inhibition of PARP2 with similar potency as well as interfere with other biological pathways involving NAD^+, which may cause toxicities like acute myeloid leukemia, myelodysplastic syndrome and GI toxicity. Overall, looking at the success rate of PARP1 inhibitors into various solid tumors, there is an urge of novel and selective PARP1 inhibitors. With the aim of designing next generation PARP1 inhibitors, a ligand based drug design approach; 3D-QSAR study was performed on a series of 2,3-Dihydrobenzofuran-7-carboxamide derivatives reported as PARP1 inhibitors. Total dataset of 31 molecules divided into training set (23) and test set (8) in 75:25 ratio. Three different alignment methods were used and amongst them distill based alignment was found to be significant. Contour map analysis of best CoMFA and CoMSIA model suggested donor, acceptor, steric and hydrophobic favourable groups as important ligand features. Eleven diversified and potent PARP1 inhibitors were used to develop a ligand based pharmacophore model using DISCOTECH module, which was refined by GASP in SybylX software. The best model generated has three types of pharmacophoric features namely, hydrogen bond donor (HBD), hydrogen bond acceptor (HBA) and one hydrophobic (HYD). The predictive power of pharmacophore model was then validated using GH score and ROC curve method. The results obtained from total of 551 dataset (51 Actives + 500 Decoy) as GH score is 0.952 and Enrichment factor (E) is 9.58. Finally, this model was screened against NCI library and total 6992 hits were obtained after applying various filters. Hits with higher Q_{fit} value were then subjected to molecular docking in the active site of PARP1 (PDB ID: 4PJT, BMN-673) and PARP2 (PDB ID: 4TVJ, Olaparib) using GOLD software. Hits with higher Gold score against PARP1 were chosen as virtual PARP1 inhibitors which can be later optimized into lead and synthesized as promising PARP1 inhibitors for the further development.

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O-20

Assessment of Implementation of Antibiotic Stewardship Program in Surgical Prophylaxis at a Secondary Care Hospital in Ras Al Khaimah, United Arab Emirates

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Abstract: Inappropriate use of antibiotics is the leading cause of development of new bacterial resistance mechanisms that are spreading globally at an alarming pace. Few studies have been carried out to assess the standard practice of care of physicians in utilization of antibioticsin UAE hospitals. This retrospective and prospective study was conducted to evaluate recently implemented antibiotic stewardship program for surgical prophylaxis at a secondary care hospital inRas Al Khaimah, UAE.The data of in patients of both gender were documented in the predesigned patient profile form and the prescribing practice of surgical prophylaxis antibiotic for clean and clean-contaminant surgical procedureswas compared and analyzed for patient's, surgical procedures', drug's therapy related parameters and percentage adherence to local hospital guidelines,two months prior and after the implementation of antibiotic stewardship program.Four hundred and ninety-three patients were included in the study, out of which 347 in preimplementation and146in post implementation period of local hospital guidelines.All medications were prescribed by their generic names. The most commonly used antibiotic was cefuroxime (161; 46.39%), followed by amoxicillin (85; 19.45%).There was no significant difference in term of antibiotic selection (p =0.553) and administration within 1 hour of incision (p =0.061)between prior and post local guidelines implementation groups, but significant difference (p= <0.0001) was observed when medications were required to be discontinued within 24 hours after the surgery. *In order to* prevent the spread of antibiotics resistance in the region, *continuous medical education and cyclic auditingshould be implemented and followed in hospitals.*

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O-21

FACILE Cu (I)-INDUCED ACTIVATION OF FURAN TO [4+2] AZA-DIELS-ALDER REACTION FOR SYNTHESIS OF TETRAHYDROPYRIDINES

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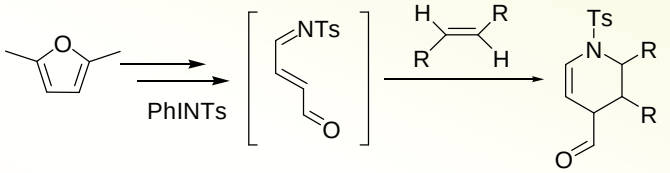
Abstract: Nitrogen heterocycles are of immense importance not only as key components of a range of bioactive compounds, both naturally occurring and synthetic, but also as synthetic precursors to a variety of pharmaceutically and industrially relevant nitrogen-containing compounds.[1] In particular,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



Scheme 1

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

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O-22

RegioselectiveSynthesis and PhotophysicalStudies of Triazolyl Boron-dipyrromethene Complexes

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Abstract: Dipyrromethane and Boron-dipyrromethenes (BODIPYs) have been persisted to get hold of incredible popularity to their simple structure, interesting and fantastic spectroscopic properties similarly to be useful as flexible fluorescent probe dyes in biotechnology subject [1].They have desirable solubility, stability towards mild and chemical substances, exhibit to relatively the excessive molar absorption coefficients and fluorescence quantum yields [2]. Moreover, spectroscopic and photophysical properties of BODIPYs can be tuned by the suitable functionalizing of the meso or α,β-peripheral core positions [3]. In continuation of our efforts to identify effective photosensitizers and fluorescent probes, we have developed a facile synthetic protocol to access diverse 1,2,3-triazolyl appendedand investigated their photophysical properties[4]. Formation of triazolylappendedBODIPYsinvolve the reaction of BODIPYs with iodine(III) reagent togenerate bodipyphenyl-iodonium salts which was *in situ* treated with sodium azidefollowed by arylalkynes.Newly prepared 1,2,3-triazolyl appended BODIPYderivativeswerefully characterized by NMR (^{1}H &^{13}C) and HRMS-TOF mass spectral data. Some of the prepared BODIPYderivatives were found to display interesting absorption and emission properties. Synthesis, characterization and photophysical studies of the triazole appended BODIPYs will be discussed in the conference presentation.

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O-23

Substrate-switched dual functionalization of alkenes: catalyst-free synthetic route for *β*-hydroxy and *β*-ketothioethers

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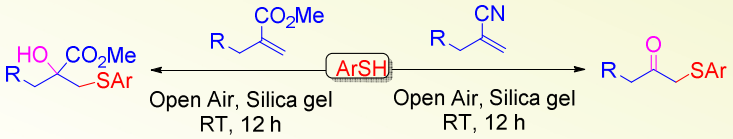
Abstract: Difunctionalization of alkenes is a fascinating method to promptly increase molecular complexity in a step-economic fashion, has emerged as a hot topic in recent years for the construction of carbon-carbon or carbon-heteroatom bonds.[1]Owing to the widespread presence of organosulfur compounds in numerous natural products, biologically active molecules and also their applications in organic and medicinal chemistry, bioconjugate chemistry, polymer science, and pharmaceutical chemistry.[2] In this study, a substrate-controlled dual functionalization of alkenes under catalyst-free and solvent-free conditions is described. Alkenes possessing different electron-withdrawing groups, namely, ester and nitrile, reacted with a variety of thiols under air to provide *β*-hydroxythioethers and β-ketothioethers, respectively, in good to excellent yields.[3]



• Catalyst Free • Solvent Free • Green Synthesis
• Excellent Yields • Room Tempterature • 32 Examples

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O-24

DEVELOPMENT, CHARACTERIZATION AND EVALUATION OF SOLID LIPID NANO PARTICLES OF *ALOE VERA*

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ABSTRACT: Background: Nowadays, the sunscreen creams are composed of mostly synthetic chemicals and other organic compounds which were found to enter into the blood stream on topical application raising concerns in the scientific community[1,2]. *Aloe vera* is a natural luscious evergreen xerophitic plant containing glucomannans, and having excellent anti-oxidant properties. The permeation effect and drug stability of the drug candidate can be significantly enhanced by formulating it into solid lipid nanoparticles (SLN).

Objective: The main objective of the study was to formulate and evaluate *Aloe vera*-loaded SLN sunscreen cream and to determine its photoprotective potential.

Methods: The *Aloe vera* loaded SLN's were formulated by microemulsification technique. The developed SLN's were studied for its entrapment efficiency, poly dispersity index (PDI), zeta potential, particle size and other characterization techniques. Finally, the optimized SLN's were incorporated into the sunscreen cream and evaluated for its spreadability, viscosity, extrudability, drug content, *in vitro* drug release, *ex vivo* permeation, *determination of* sun protection factor, and accelerated stability studies[2,3,4].

Results: The formulated nanoparticle showed low PDI with optimum zeta potential for sufficient stability with adequate entrapment efficiency. The *in vitro SPF was found out to be* 16.9±2. Stability studies were performed under accelerated conditions and no appreciable changes in the parameters were noticed.

Conclusion: The solid lipid nanoparticles of *Aloe vera* were incorporated into a cream and the SPF of the resultant sunscreen cream was found to be on par with the sunscreens that were currently available in the market.

Keywords: photoprotective, phytobioactive, *Aloe vera*, solid lipid nanoparticles, UV, sunscreen cream

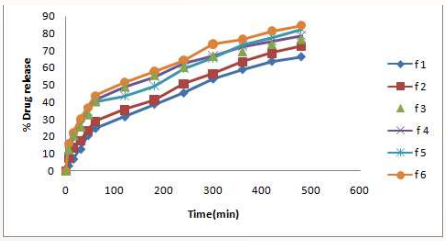

Fig 1: *In vitro* drug release profile of sunscreen formulation (F1- F6)

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O-25

Enantio- and Diastereoselective Two-Pot Synthesis of Isoquinuclidines from Glutaraldehyde and N-Aryl Imines with DFT-Calculations

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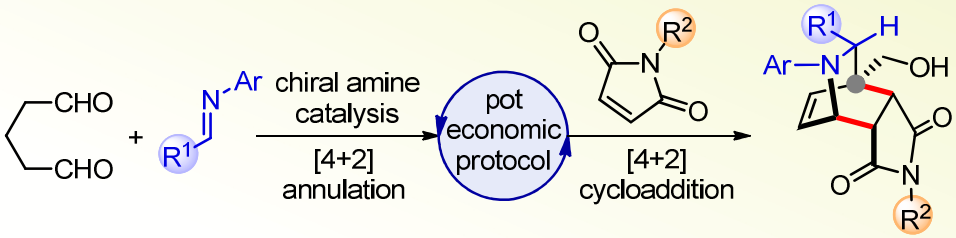
Abstract: The 2-azabicyclo[2.2.2]octane, isoquinuclidine is an attractive scaffold found in numerous bioactive natural and unnatural products.[1] This structural unit also serves as a building block for additional functionalizations to access natural products scaffolds, and other drug molecules like Tamiflu,[2] which is an essential anti-influenza drug. Given such potential importance, the development of methods for asymmetric synthesis of isoquinuclidine has gained much interest, and reviewed recently.[3]In continuation of our study towards the use of lineal dialdehydes for the synthesis of medium sized N-heterocycles,[3] we recently developed an efficient organocatalytic asymmetric method for the synthesis of 1,2-Dihydropyridines (DHPs).[4]Here, we extended this chemistry to access 2-azabicyclo[2.2.2]octane "Isoquinuclidine" systems in 'pot-economic' fashion with high yields (up to 78%) and excellent stereoselectivity(>50:1 dr, and up to >99:1 er) with overall five-steps(Scheme 1). DFT-calculations supports the observed high stereoselective reaction outcome.[5]



- *metal-free, five-steps, and two-pot protocol with DFT calculations*
- *endo-product exclusively with five-contiguous chiral centers*
- *yields (up to 78%) and stereoselectivites (>50:1 dr, up to 99:1 er)*

Scheme 1: Pot-economic synthesis of 2-azabicyclo[2.2.2]octane 'isoquinuclidine' system

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O-26

A novel attempt to explore the pharmacophoric space of the enzymatic proteome of *Plasmodium falciparum* using multicomplex-based pharmacophore modelling

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Sub Areas/Main Topics: Structural Biology and Bioinformatics Research
Presenting Author: Anu Manhas (01/03/1991)

Abstract:

Background: Number of molecules has been crystallized against the potential targets of *Plasmodium falciparum* to describe the structural basis of inhibition. However, the pharmacophore studies accomplished so far have not included all the interaction patterns. Thus, we made a retrospective analysis of pharmacophores mapped from the 16 classes of *Pf* structural proteome and identify the unique patterns that can be employed for drug design.

Observation: It was observed that most of the inhibitors have shown affinity for the off-targets. Thus, it seems that none of the model has the capability to screen its own experimental known inhibitors. A wide range of values were retrieved for the specificity, sensitivity, area-under-curve receiver-operating-characteristic, Enrichment-factor and Güner-Henry. However, out of the 16 *Pf* enzymes, Plasmepsin-2 and Orotidine-5'-phosphate-decarboxylase were the only two enzymes that have the capability to differentiate between the actives and inactives. Pharmacophore clustering revealed that similarity in the pharmacophore pattern is accountable for the haphazard screening of the inhibitors. Also, fingerprinting-based ligand similarity search method retrieve that >50% of similarity was reported between the mapped actives and presumed inactives. However, some targets haven't shown much significant similarity due to incapability of the pharmacophore to retrieve its own actives and also owing to the intricacy in the pharmacophore features.

Conclusion: The combined clustering and ligand-similarity search approach revealed the efficiency in recognizing the pharmacophore pattern for the construction of the stringent pharmacophores of *Pf* proteome that can be utilized for the virtual screening.

O-27

Synthesis of Entecavir-Aristeromycin Hybrid Scaffold as anti-HBV Agents

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Abstract: Hybridizing the major motif of entecavir and aristeromycin, novel carbocyclic nucleosides were synthesized. Introduction of 4'-alpha methyl and 7-deaza base were chosen to evaluate their effect on antiviral activity against Hepatitis B virus (HBV). The novel carbocyclic sugar key intermediate was efficiently synthesized as a single diastereomer from D-ribose. The key step was established *via* BINAP-Rh(cod)$_2$BF$_4$ catalyzed reductive carbocyclization of 1,6-enynes.Mitsunobu reaction was utilized to yield protected carbocyclic nucleosides.Subsequent deprotectionfollowed by aminolysis yieldedthe target entecavir-aristeromycin hybrid analogues.All the synthesized compounds were evaluated for their anti-viral properties against HBV. One of them exhibited potent anti-HBV activity (EC_{50}= 3.4 μM) without significant cytotoxicity (CC_{50} = 87.5 μM). These findings from the present work warrant the way for future investigation as well as additional biological evaluation of this novel class of carbocyclic nucleosides.

Key words: Entecavir, Aristeromycin, Anti-HBV,Mitsunobu coupling.

O-28

Highly Atom-Economic, Catalyst-free, and Solvent-free Phosphorylation of Chalcogenides

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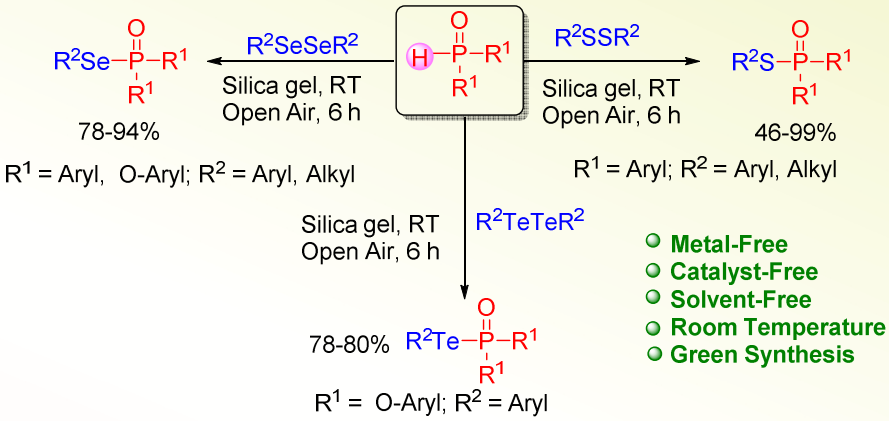
Abstract: The organic frameworks possessing both sulphur and phosphorus moieties play important role in organic synthesis, pharmaceuticals, materials, medicinal chemistry and agrochemicals.[1-2]Here we described afacile silica gel promoted, catalyst-free and solvent-free synthesis sulfophosphorus compounds *via*S-P, Se-P and Te-P bond formations. Variety of disulfides coupled with diarylphosphine oxides to provide the corresponding phosphinothioate in excellent yields. For the first time, diselenides and ditellurides reacted with dialkylphosphites under catalyst-free conditions to provide the corresponding phosphoroselenoate and phosphorotelluroate respectively in good to excellent yields.



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O-29

Development of Modified MacMillan based Ionic liquids as organocatalystfor Asymmetric Friedel-Crafts Reaction

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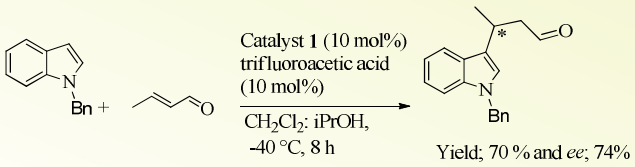
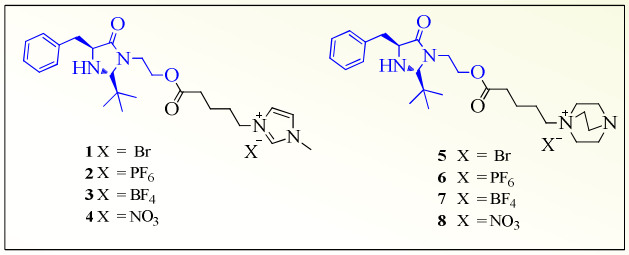
Abstract: Over the last two decades organocatalysisbecome a suitable and powerful strategy for various asymmetric transformations. The Fridel-Crafts reaction is one of the most powerful methods for the formation of a new C-C bond and has been widely utilized in industrial processes [1-4].We have developed a chiral ionic liquid of modified MacMillan catalyst (1-8) from the reaction of bromoester and DABCO or 1-methyl imidazole. The Asymmetric Friedel-Crafts reaction of 1-benzylindoleand crotonaldehyde gave 3-(1-benzyl-1H-indol-3-yl)butanal with 70% yield and 74% *ee*by using modified MacMillan based chiral ionic liquid **1** (10 mol%) and trifluoroacetic acid (10 mol%) at -40°C in dichloromethane:isopropanol(85:15) solvent.





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O-30

LigTMap: Ligand and Structure-Based Target Identification and Activity Prediction for Small Molecules

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Abstract: To facilitatethe drug discovery process, we present LigTMap as a one-stop server fortarget identification, pose prediction, and binding activity prediction of 25 pharmacologically relevant target classes. The prediction methodadopts a two-stage approach. It firstly identifies potential targets of a query compound by ligand fingerprint (Morgan+MACCSF) similarity analysis. Then, it performs PSOVina docking to each potential target and associates the binding pose of the query compound to that of the crystal ligandthru SIFT binding fingerprint.The collective scoring of ligand and binding fingerprint identified the target. We assessed LigTMap against a validation dataset comprising of 730 compounds from 7 targets and an independent test dataset comprising of 100 compounds from 6 targets. Remarkably, the validation resultdisplayed that LigTMap findsthe correct targets in 48.15%, 62.34%, and 65.48% of the cases in the top 1, top 5, and top 10, respectively. For the test dataset, LigTMap performs superior to SuperPred and HitPick, while it performs on par with Swiss Target Prediction and SEA. For binding activity prediction, our RF models have an average Pearson's correlation coefficient of 0.73 in nested cross-validation and 0.75 in the test of an independent dataset. Overall, LigTMap is a comprehensive target identification server that predicts straightaway the relevant PDBs of targets for query compounds. Currently, it supports the identification of 5000 protein targets and is available freely for academic and researchpurposes at https://cbbio.cis.um.edu.mo/LigTMap/.

O-31

Visual Detection of Aqueous Health Hazard Ions

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Abstract: Some metal ions (Al^{3+})and nonmetal ions (F^-) are health hazard, found abundantly in the environment. Although many methods have been reported for the efficient detection of these toxicants, an easy and accessible sensor for fast detection of aqueous toxicants have not been developed to date.We havesynthesisedsilver nanoparticles for the detection of metal ionsin the presence of potential interfering metal ions [1].Our research grouphas also developed visual sensor for the sensing of fluoride from aqueous system [2]. The sensitivity of the detection probe has been optimised by variations in size and distribution of nanoparticles. Moreover, the developed nanosensors can also be applied to trace metal contamination in different types of water samples. The economic viability of synthesized nanomaterials, in comparison to other available materials, is evident from the cost-benefit analysis.

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O-32

Ultrasound promoted synthesis of Novel benzothiazinone derivatives and its pharmacological evolution

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Abstract: The benzothiazinone lead compound, BTZ043, kills Mycobacterium tuberculosis by inhibiting the essential flavo-enzyme DprE1, decaprenylphosphoryl-beta-D-ribose 2-epimerase. In search of new active molecules against Mycobacterium tuberculosis, herein, we report aultrasound promoted synthesis of substituted BTZs bearing a variety of different substituents at the C-2 position. Compounds were screened for their *in vitro* antibacterial, antifungal and also antimycobacterial activity against Mycobacterium tuberculosis H37Ra and asmall focused library of benzothiazinone via Green chemistry approach. Structures of all newly synthesized compounds were characterized by their Mass, IR, ^{1}H &^{13}C NMR and Elemental analysis.

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Keywords: Nitrobenzothiazinone (BTZ), *In vitro* Antibacterial, Antifungal, Antimycobacterial activity, Mycobacterium tuberculosis $H_{37}Ra$.

O-33

PPE2: a blessing in disguise

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Abstract: PPE2 is a member of the PPE family of proteins in *Mycobacterium tuberculosis*. Previous studies have shown that PPE2 inhibits nitric oxide production in macrophages by specifically binding to TATA box of iNOS promoter. We observed that, during infection in mice, Mycobacterium smegmatis expressing PPE2, reduced tissue resident mast cells. Since, mast cells are major players in inflammation, we tested recombinantly purified PPE2 (rPPE2) as an anti-inflammatory agent. In formalin-induced paw inflammation, mice treated with rPPE2 showed reduction in edema and mast cell population. Presence of a "TAT protein" like motif in PPE2 enables its energyindependent uptake in tissue fibroblasts. Further, KitL; a fibroblast cytokine that regulates tissue mast cells, was found to be transcriptionally downregulated in rPPE2 treated mice. Also, unlike a majority of the NSAIDs, rPPE2 did not cause any renal or hepatotoxicity. Therefore, rPPE2 emerges as a novel therapeutic for the treatment of inflammation, with no apparent side effects.

O-34

Isolation, screening and molecular characterization of multidrug resistant organisms, to screen and identify carbapenem producers, from operation theaters and Intensive Care Unitsof Ahmedabad.

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Abstract: In depth evaluation of the organisms isolated from critical care area is of epitome importance in order to prevent or control hospital acquired infections. As per the CLSI guideline, identifying organism and finding out antibiotic resistance pattern not only help one to understand the epidemiology of hospital acquired infections, but it also helps in formation of robust strategy to fight the menace. In the current study, operation theaters and intensive care units were screened as per the international guideline, using air sampler and through surface swabbing. All the isolates were identified; antibiotic susceptibility testing was carried out, furthermore, multidrug resistant isolates were subjected to confirmatory tests to screen carbapenem resistance. Genetic screening using real time PCR was performed on the isolates to rule out the gene responsible for imparting the resistance. Contradicting to the anticipation, out of 2304 samples screened, 103 surface swabs showed multidrug resistant strains; whereas, 89 air samples showed presence of multidrug resistant organisms. Further screening revealed that less than ten isolates were carbapenem resistant. Complimenting to the above tests, genetic analysis for responsible genes showed presence of KPC gene in three isolates. Hence, it is evident from the study that, every single isolated organism has to pass through the rigorous screening procedure and presence of multidrug resistant strain must result into complete evacuation and thorough inspection of the area to rule out and irradiate the source.

O-35

8-HYDROXYQUINOLINE-SULFONAMID HYBRIDE LIGAND AND ITS METAL CHELATES: SYNTHESIS, CHARACTERIZATION, *IN SILICO* ADMET, *IN VITRO* ANTIMICROBIAL, DNA INTERACTION AND MOLECULAR DOCKING STUDIES

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Abstract: Sulfonamide groups are now added to known biologically active scaffolds to generate new effects. Here 4-amino-N-(8-hydroxyquinolin-5-yl)benzenesulfonamide (8HQBS) a sulfonamide based 8-hydroxyquinoline derivative was synthesized as a scaffold to generate its Cu(II), Ni(II), Zn(II), Mn(II),Co(II) and Fe(II) metal chelates. The structural features of 8HQBS ligand was elucidated by MASS, FT-IR, ^{1}H-NMR, ^{13}C-NMR and its metal chelates by studying their physiochemical properties, elemental analysis, FT-IR, thermogravimetric analysis, UV-Visible and magnetic susceptibility. These data explains presence of two water molecules in the coordination which gives the idea of octahedral geometry of synthesized complexes. *In silico* ADMET studies was carried out by Swiss ADME and Osiris datawarrior. Molecular docking studies was carried out on bacterial proteins (PDB ID: 5h67, 3ty7, 3t88 & 5i39) and double helix DNA (PDB ID: 1BNA) the results are represented in terms of binding affinity. Antibacterial properties were experimentally validated in the form of minimum inhibitory concentration. The results showed increased biological activity of free ligand on metal complexation. Also interaction of complexes with CT-DNA was carried out by viscosity measurement, electronic absorption titration and gel electrophoresis and the results showed intercalation binding mode.

Keywords: sulfonamide, 8-hydroxyquinoline, antibacterial, DNA binding, ADMET, molecular docking

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O-36

Direct Use of Sugarcane bagasse derived hemicellulose hydrolysate for the synthesis of *C*-glycosyl derivatives by the Lubineau Reaction

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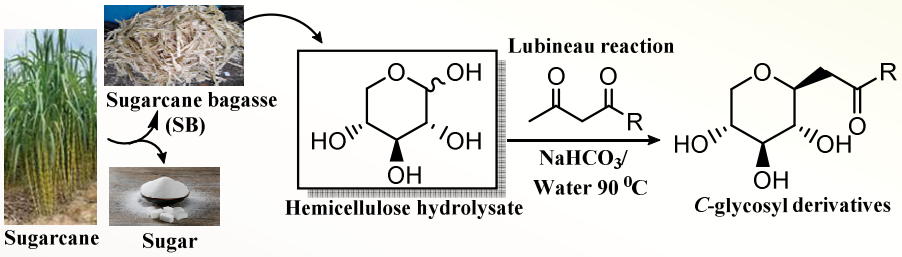
Abstract: *C*-glycosyl derivatives have gained a huge interest in recent years as these molecules are used as therapeutics, bioactives, bioactive candidates, probes, synthons, and building blocks. Some pioneering chemical methods for their synthesis involve the C-C bond formation at the anomeric carbons or hemiacetal carbons of unprotected sugars, which basically include reactions of sugars directly or via in situ-formed imines/iminium ions, with nucleophiles.[1,2] The problem to access such class of compounds according to the principles of green chemistry was a great challenge when embraced by Professor Lubineau.[3] One of the most well-known application of the Lubineau reaction is easy access of *β*-*C*-xylopyranosylpropan-2-one which is a precursor of Pro-Xylane-an effective activator of glycosaminoglycans biosynthesis and play a major role in the organization of extracellular dermal matrix and in skin hydration.[4,5]

Lignocellulosic biomass is a promising substitute for the fossil fuels and its utilization in a green and effective way is of great importance for sustainable development bio based products. The Indian Sugar Industry crushes annually about 225-250 MT of sugarcane thereby generating nearly 40-44% of lignocellulosic biomass residue i.e. 90-100 MT sugarcane bagasse and trash. This low value biomass feedstock remains underutilized to a great extent in the context of commercialization of agro-residues biorefinery. Herein, our research was undertaken to investigate the potential utilization of sugarcane bagasse derived hemicellulose hydrolysate as a substitute of pure xylose in the Lubineau reaction (Scheme 1). Our preliminary results indicate that the hemicellulose hydrolysate can be used directly as xylose feedstock to afford *C*-glycosyl derivatives.



Scheme 1

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O-37

REGULATORY COMPLIANCE MANAGEMENT OF TRANSDERMAL PATCHES

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ABSTRACT: Regulatory affairs (RA) professionals play critical roles in a pharmaceutical industry because it is concern about the healthcare product lifecycle, it provide strategic, tactical and operational direction and support for working within regulations to speed up the development and conveyance of safe and effective healthcare products to individuals around the world. Regulatory compliance is adherence with different laws, regulations, guidelines and specification relevant to process. Violation of such regulations may prompt lawful disciplines. Regulatory compliance describes the goal that organizations aspire to accomplish in their efforts to ensure that they are aware of and take steps to fulfil with relevant laws, policies, and regulations. The pharmaceutical industry is highly regulated industries in our country and is dealing with human life, so adherence with the regulation and regulatory guidelines must require. Transdermal Patches are now becoming widely used drug delivery system. The current scenario shows that the ration of generic drug is double than new drug. Transdermal Patches are at the third place after oral and Injectable in the category of widely used pharmaceutical products worldwide. There are only 54 Transdermal patches available in the market from which 28 are new patch and 26 are generics. Drug delivery systems plays crucial role in Pharmaceutical Research and Development. To promote the efficiency of drug and extend the life cycle of product, quantitative analysis of approval process and knowledge of the technical barriers must require.

KEYWORDS: Transdermal Patch, Guidelines & Regulation, Lifecycle Management, Regulatory Compliance

POSTERS

P-1

Understanding of correlation between Proteolytic systems and Myogenic regulatory factors: Fundamental determinants for myogenesis

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Abstract: Chronic diseases (cancer, diabetes, COPD) are associated with increased inflammatory and oxidative species related stress to the body. The level of these stress molecules beyond threshold value has been associated with alteration in skeletal muscle protein metabolism and leads to loss in muscle mass (atrophy/wasting). Such metabolic condition under chronic diseases sometime becomes the key reason for human morbidity and mortality. Thus understanding the etiology of atrophy may help to improve the quality of life. Myogenesis is process which helps the muscle fibers to get repaired during any damage but under diseases conditions (such as duchenne muscular dystrophy) repair process is overtaken by damage which further contribute in the atrophy. Although proteolytic systems are reported to be upregulated under any atrophic conditions and inhibition of these systems prevent the protein degradations and protects the muscle fibers yet complete inhibition may also hampers the myogenesis process. Thus to understand the etiology of atrophy, understanding of phenomenon of myogenesis is essential. In the present study, diverse stages of cells were collected during myogenesis by using C2C12 cell lines (*i.e.* reserve cell, 50% myoblast and different differentiation stages from 0h-120h) and cytohistochemistry, biochemical assay, qRT-PCR and immunoblotting were performed to study the diverse proteolytic systems and myogenic regulatory factors (MRFs). Data illustrate that 5 key proteolytic systems (cathepsin L, calpain, caspase 3, Ub-proteasome and autophagy) express in orchestral manner with key MRFs (*i.e.* Myf5, MyoD, myogenin, MEF2D, MRF4 and Pax7) which concomitantly determine the fate of myogenic progenitor cells. Such data illustrate that these proteolytic systems and MRFs are related to each other and have some correlations which further need to be explored. So, in-depth understanding of these fundamental determinants may illustrate the process of myogenesis and eventually would contribute in improving atrophy.

Keywords: C2C12 myotubes, MRF, proteolytic systems, myogenesis, atrophy

P-2

Efficient and modified fluorescent based glucose uptake assay to study skeletal muscle insulin resistance induced under diverse stresses in cultured myotubes

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Abstract: Uptake of glucose is an important phenomenon for cell homeostasis, and assay to study this uptake is one of crucial parameter required for exploring diverse metabolic disorders such as diabetes mellitus, myocardial ischemia and cancer. Skeletal muscle being the largest organ of the body is responsible for more than 75% of glucose disposal in response to insulin and contraction. Under type-2 diabetes, a primary defect in skeletal muscle is the insulin resistance and to study such disorder measurement of glucose uptake is a fundamental requirement. Various approaches including use of scintillation counter, flow cytometer, fluorometer and spectrophotometer are being employed by researchers to quantify glucose uptake in the cell with the help of radio- and fluorescent-labelled molecules. One of the most popular molecules is the fluorescent labelled glucose analogue *i.e.* 2-NBDG. Though 2-NBDG based glucose uptake assay is the majorly used approach in various cells including skeletal muscle even then its protocol is either not reported well or not reproducible as demonstrated in the literature. No significant difference was observed in insulin stimulated C2C12 myotubes compared to control using diverse available protocols. Thus in present article, using muscle specific cells i.e. mouse skeletal muscle derived C2C12 myotubes,we re-established the fluorescence (2NBDG)-based protocol and explored its efficiency to study insulin resistance induced under diverse (oxidative & inflammation) stress conditions in cultured myotubes. Our present protocol is very efficient, effective and improvised for studying the glucose uptake in skeletal muscle cells specifically under inflammation and oxidative stress-induced insulin resistance conditions.

Keywords: 2-NBDG, assay, Insulin resistance, C2C12 myotubes

P-3

Anti-atrophic potential of butylated hydroxytoluene (BHT) under H_2O_2-induced stress in C2C12 myotubes: Repositioning of a well known antioxidant

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Abstract: Increased oxidative stress is one of the key factors for diverse chronic diseases (cancer, diabetes, COPD) mediated consequences including alteration in protein metabolism that result in loss in skeletal muscle mass (atrophy/wasting). Studies show under such clinical settings, uncontrolled atrophy itself becomes the reason for human morbidity and mortality. Till date no therapy is available or recommended for atrophy by the FDA (USA). Available reports show that BHT, a synthetic antioxidant widely used as food additives, is reported to protect cells from pathological impact induced during diverse clinical settings (cancer, cardiovascular disorders and aging) by maintaining the redox status of cells. Studies also show that BHT inhibited the protein degradation induced by proteolysis-inducing factor and high glucose level in cultured myotube, which prompted us to hypothesize that BHT administration protects the skeletal muscle fibers against H_2O_2 induced atrophy. In the present study, mouse skeletal muscle derived C2C12 myotubes were treated with H_2O_2 (100□M) in the presence or absence of BHT (25□g). Our histocytochemical and biochemical studies show that BHT pre-administration (4h) protects the myotubes morphologically (*i.e.* length, diameter and fusion index) by preventing its leakage (CK and LDH release) due to oxidative stress induced by H_2O_2. Molecular data also illustrate that BHT treatment prevents the degradation of muscle specific protein (MHCf) induced due to atrophic impact of H_2O_2 which elaborate the protective effects of BHT in the H_2O_2 treated myotubes. Overall our preliminary study provides the first direct evidence of protective effect of BHT on cultured myotubes atrophy.

Keywords: BHT, Muscle atrophy, Oxidative stress

P-4

Synthesis, spectroscopic, thermal and In-vitro biological screening of some novel Cr(III) based heterochelates

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Abstract: In present work novel pyrazolone based organanic semicarbazone derivatives and their spectroscopic and biological activities were investigated. A new series of pyrazolone based semicarbazone ligand and their Cr(III) heterochelate were synthesized. The structure of semicarbazone ligands were confirmed by ^{1}H NMR, IR, Elemental analysis and their heterochelates were confirmed by thermal studies (TGA/DTG & DSC) and FAB Mass spectroscopy. All the synthesized compounds were screened for their In-Vitro biological screening against $Gram^{+ve}$ and $Gram^{-ve}$ microorganism. The results confirmed that semicarbazone based heterochelates have a great potential and significant for further investigation.

Keywords: Semicarbazone, Pyrazolone, Cr(III) heterochelates, Thermal studies, Biological studies.

P-5

Synthesis of steroidal dihydropyrimidine by ultrasound irradiation

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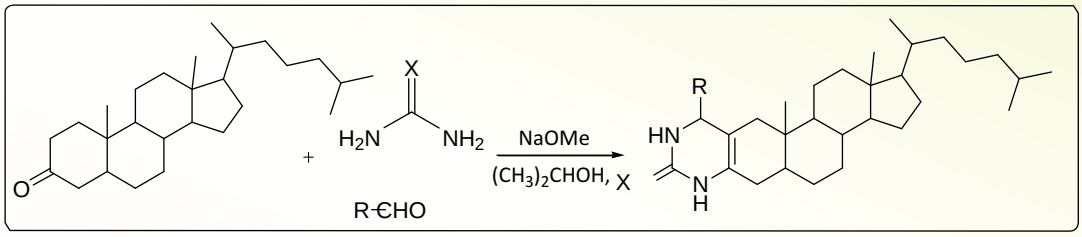
Abstract: Aryl-3,4-dihydropyrimidinones have recently received great attention because of their wide range of therapeutic and pharmacological properties, such as antiviral, anti-tumor, antibacterial andantiinflammatorybehaviour.[1]Furthermore,thesecompoundshaveemergedastheinte-ralbackbones ofseveralcalciumchannelblockers,Antihypertensive,α-1a-adrenergicantagonists,andneuropeptideY (NPY) antagonists. [2] Moreover, several alkaloids containing the dihydropyrimidine unit have been isolated from marine sources, which also exhibit interesting biological properties. [3] Thus, synthesis of thisheterocyclicnucleusisofmuchcurrentimportance.Accordingly,manysyntheticmethodshavebeen describedintheliteratureHowever,inmanycases,expensiveandtoxicmetals,extendedreactiontimes, and/orelevatedreactiontemperaturesarerequired,providingopportunityforthefurtherdevelopmentof milder protocols. In continuation of our interest on the facile synthesis of steroidal 3, 4-dihydropyrimidine-2(1H)-thione/one using mild conditions, we accomplished a convenient route to synthesis of dihydropyrimidinone in presence of NaOMe under ultrasound radiation. Here in we report an efficient simple method for synthesis of the new steroid-dihydropyrimidine derivative,using a three component system in presence of sodium methoxide from steroidal carbonyl compound, aliphatic/aromatic aldehyde and thiourea/urea inisopropanol.



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P-6

Synthesis of novel Benzoimidazopyrazine scaffolds via in-situ decomposition of DMF

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Abstract: Imidazo-pyrazines are an intriguing structural motif that are ubiquitous in bioactive molecules and drug discovery.[1] The diverse biological/pharmacological potency of imidazo-pyrazines are well documented. Molecules containing the imidazo-pyrazine core have exhibited remarkable potency as a hypoglycaemic, anti-inflammatory, antihypertensive, inotropic, antiulcer, antibronchospastic, anticancer, antimalarial, uterine relaxant agent, cyclic nucleotide phosphodiesterase inhibitor, and kinase inhibitor.[2] Moreover, they are also known to manifest fascinating photo-physical properties such as chemiluminescence and bioluminescence. Owing to their diverse biological and pharmaceutical potency, this nitrogen containing polynuclear heterocyclic scaffold has attracted immense attention from both chemists as well as biologists.[3] In our present research, a group of benzo[4,5]imidazo[1,2- a]pyrazine have been synthesised from appropriate starting materials by condensation of a benzoimidazo scaffold with α-halo ketones followed by cyclisation of the keto moiety. The reactivity of the heterocycle was explored through diverse reactions.

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P-7

IN SILICO TARGET IDENTIFICATION STUDY OF NOVEL ANTI-LEISHMANIAL AGENTS

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Abstract: Leishmaniasis is a group of parasitic diseases caused by more than 20 species of protozoan belonging to the family kinetoplastida and genus Leishmania. They are categorized into three types, out of which visceral leishmaniasis is the fatal one most prevalent in 5 countries- India, Bangladesh, Nepal, Sudan, and Brazil [1]. Since there is no vaccine available for its prevention, the treatment solely depends upon the decade-old chemotherapy. However, the currently used drugs have significant setbacks in the form of toxicity, price, feasibility, and the possibility of gaining resistance, thus limiting their potential. Beta-carbolines are a class of compounds that have wide pharmacological applications, as reported by several researchers [2]. They also have been reported to possess potent anti-leishmanial activity. However, only a few reports shed light on the mechanisms by which they act [3,4].Hence in the present study, an effort has been made to identify the target(s) by which they act by *in silico* molecular docking studies using Molegro virtual docker 6.0. Significantly active compounds found out by our research group were docked against well-known targets- trypanothione reductase (PDB ID-5EBK) and pteridine reductase (PDB ID-1E7W). The docking results revealed that trypanothione reductase might be a putative target for titled beta-carbolines. Among the titled analogs, compounds 1d and 4d exhibited Moldock scores of -104.359 and -105.118 respectively while the co-crystallized ligand exhibited Moldock score of -61.1485. Compound 4c exhibited vital interactions with the active site residues Cys52, Cys57 and His461 involved in the catalysis further emphasizing that trypanothione reductase may be a putative target for the titled beta-carbolines
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Keywords: Leishmaniasis, beta-carbolines, trypanothione reductase

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P-8

Interaction study of Artemisinin with Bovine Liver Catalase: A biophysical and computational study

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Abstract: Many of the diseases afflicting people are attributable to oxidative stress that results from an imbalance between formation and neutralization of free radicals [1]. These free radicals,produced both endogenously and exogenously initiate oxidative stress in healthy human cells by causing lipid peroxidation, protein and DNA damage which contribute to numerous pathological diseases including cancer, atherosclerosis, cardiovascular diseases, ageing and inflammatory diseases [2]. Artemisinin, a sesquiterpene lactone obtained from *Artemisia* annua (*A. annua*,), is highly effective and promising drug has been widely used in the treatment of malaria by targeting *Plasmodium falciparum.* Hence,*A. annua*, a rich source of antioxidant flavonoids plays an important role in potentiating the effects of Artemisinin drug against diseases caused by alteration in antioxidant system. The correlation was established between free radicals and Artemisinin toxicitywhere increased activity of antioxidant enzymes is in agreement with free radicals scavenging capability of *A. annua*plant due to highly active antioxidant defence system. Therefore, the unaltered and increased catalase activity is due to resistance towards Artemisinin was reported in astrocytes cells [3]. In this investigation, we studied the effectiveness of Artemisinin in Bovine liver catalase (BLC) is one of the major antioxidant enzymes which is used to detoxify the harmful effect of free radicals that is one of the principal causes of oxidative stress. The study was accomplished by using spectroscopic methods such as UV-Vis, fluorescenceand circular dichroismspectroscopy. Furthermore, Isothermal titration calorimetry and computational modelling revealed the binding mechanism through which Artemisinin binds to the BLC.

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P-9

Regioselective synthesis and X-ray crystallographic studies of biological active isoxazole acid analogs.

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Abstract: Human Immunodeficiency Virus (HIV) causes Acquired Immune Deficiency Syndrome (AIDS) and interfere with body's ability. No cure exists for AIDS but strict adherence to antiretroviral regimes can dramatically slow the disease's progress and can prevent secondary complications. It was found that Antiretroviral Therapy (ART) leads to an increased morbidity and compromised quality of life in HIV patients. This issue demand newer scaffolding for promoting alternate mechanism. HIV-1 rapidly acquire resistance to multiple drugs by mutation, which lead to treatment failures.Targeting host factors is a complementary strategy for the development of new antiviral drugs. In our endeavor towards the development of effective anti-HIV therapeutics, isoxazole compound was found to have a marked effect in treating multiple diseases, including anticancer, antimicrobial, anti-inflammatory, etc. Hereby we report the regioselective synthesis of isoxazole acid analogs via intramolecular and intermolecular ring transformation of CN isoxazole. And the single crystal X-ray crystallographic study confirms the regioselectivity of the compound.

P-10

METALLIC GOLD BASED NANOSYSTEMS IN TREATMENT OF ADVANCED STAGE ORAL CANCER

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Abstract: Head and neck carcinoma, is one of the highest prevalent cancer among men in India and ranks second in terms of mortality considering both the sexes in India as per the Globocan statistics. Most individuals exhibit oral squamous cell carcinoma (90%) due to habits like tobacco chewing, smoking, alcohol consumption, etc.The advanced stage oral cancer (Stage III and Iva) is responsible for majority of deaths and shows poor overall survival. The combined modality treatment including radiotherapy, surgery and chemotherapy used in this stage of clinical setting has lot of side effects and exhibits patient non-compliance. Therefore, multimodal targeted approach is the need of an hour.Radiotherapy often damages the neighbouring healthy cells, so dose reduction is often required without compromising the efficacy of treatment. Use of hyperthermia using gold nanoparticles has emerged as potent approach to radiosensitize cells via hyperthermia and decrease the dose of drug. Also, gold is an inert metal and its nanoparticles are easy to prepare (reduction), get small size (5-30nm), surface modify using ligands and contrast agents. The current market scenario has only one injectable monoclonal antibody approved as targeting agent for cancer which shows variable progression free survival and overall survival and also poses issue of allergic reactions and is expensive. Combining gold nanoparticles with targeted anticancer drugs can overcome the drawbacks of conventional anticancer agents which mostly are the toxic side effects to healthy cells. The combined multimodal system can serve as a platform by aiding in adjuvant therapy and help in decreasing the dose drugs used in existing treatment options. Thus, metallic gold nanoparticles can be an ideal solution to cancer therapy and act as a boon in coming years with its tremendous multifunctional and multi-modal properties,provided the research takes into consideration the toxicity, process manufacturing, cost and regulatory aspects. The present review emphasizes on development of metallic gold nanoparticles with its opportunities and applications in treatment and diagnosis of advanced stage oral cancer.

P-11

Stability Indicating HPLC Method for Determination of Riociguat in bulk and Pharmaceutical Dosage form

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ABSTRACT: A simple, specific, accurate and stability-indicating reversed phase high performance liquid chromatographic method was developed for determination of Riociguat , using a Inertsil ODS-3 C_{18} column and a mobile phase composed of buffer : ACN (50:50, v/v), pH 5.0 adjusted with glacial acetic acid. The retention time of Riociguat were found to be 5.6 mins. Linearity was established for Riociguat in the range of 1.00-3.00 µg/ml. The Accuracy was found to be 99.8%. The drug was subjected to Acid and Alkali hydrolysis, oxidation, thermal and photolytic degradation. The degradation studies indicated, Riociguat to be susceptible to acid and alkaline hydrolysis. This method can be successfully employed for routine analysis of Riociguat in bulk and formulations.
Keywords: Riociguat, stress testing, stability indicating method, HPLC.

P-12

DEVELOPMENT AND VALIDATION OF A STABILITY INDICATING RP-HPLC METHOD FOR EDOXABAN TOSYLATE MONOHYDRATE USING QBD APPROACH.

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ABSTRACT: QbD (Quality by Design) has gained importance in the analytical method development. It involves the optimization of the critical parameters and to evaluate their effect on the critical quality attributes. An attempt was to develop and validate a stability indicating RP-HPLC method for the quantification of Edoxaban tosylate monohydrate in bulk form. The Box- Behnken design was used for the QbD approach in which the screening was done on the critical parameters i.e (Buffer pH, %ACN and flow rate) and their effects on the variable responses i.e (Retention time, NTP and Asymmetry factor) was evaluated. The developed method was validated according to International Conference on Harmonization guideline with respect to accuracy, precision, specificity, linearity, solution stability and system suitability. For this, an isocratic condition of mobile phase comprising buffer of 0.01 M sodium acetate with pH 4.0 and acetonitrile in a ratio of 70:30, v/v at a flow rate of 1.0 mL/ minute over Qualisil BDS C18, 250 mm×4.6 mm×5 µm column at 28°C temperature was maintained. The detection was done using a PDA detector at 290nm. The method showed excellent linear response with correlation coefficient (R2) values of 0.999 for Edoxaban tosylate monohydrate, which was within the limit of correlation coefficient (R2 ≥ 0.995). The percent recovery was found within the acceptance limit of 98.0% to 102.0% .The %RSD for precision studies was found to be less than 2%.The Limit of Detection (LOD) and Limit of Quantification (LOQ) was found be 0.2µg/ml and 0.5 µg/ml respectively.

Keywords: Edoxaban Tosylate Monohydrate, Stability indicating method, Validation, QbD

P-13

METHOD DEVELOPMENT AND STABILITY STUDY FOR VORTIOXETINE HBR USING HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

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ABSTRACT: A simple, specific and stability indicating high performance liquid chromatographic method was developed for determination of Vortioxetine HBr, using a Inertsil ODS-3 C_{18} column. The mobile phase composed of Buffer : ACN (40:60, v/v), pH 4.5 adjusted with glacial acetic acid. The retention time of Vortioxetine HBr were found to be 4.2 mins. The detection was done using a PDA detector at 228nm. Linearity was established for Vortioxetine HBr in the range of 2.5-7.5 µg/ml. The method showed excellent linear response with correlation coefficient (R2) values of 0.996. The Limit of Detection (LOD) and Limit of Quantification (LOQ) was found out. The drug was subjected to Acid and Alkali hydrolysis, oxidation, thermal and photolytic degradation. This method can be successfully employed for routine analysis of Vortioxetine HBr in bulk and formulations.
Keywords: Vortioxetine HBr, linearity, stability, HPLC.

P-14

First biocatalytic Groebke-Blackburn-Bienaymé multicomponent reaction: Highly green and efficient synthesis of Imidazo[1,2-a]pyridine derivatives

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ABSTRACT: Imidazo[1,2-*a*]pyridine is a valuable framework found in a number of nitrogen-bridgehead fused heterocycles having diverse biological activities such as antiviral, antifungal, antiparasitic anti-inflammatory and anti-cancer. However, there are numerous conventional method have been developed over the years to synthesize Imidazo[1,2-*a*]pyridine. In this context, Groebke-Blackburn-Bienaymé multicomponent reaction (GBB-multicomponent reaction), which takes place between an aldehyde, 2-aminoazine, and an isocyanide to synthesize Imidazo[1,2-a]pyridine framework in presence of numerous catalyst including Brønsted acids, Lewis acids, solid-supported acids, organic bases and ionic liquids. But these methods have some drawbacks like commercially unavailable monohalogenated compounds , toxic catalysts, less yield and long reaction time. Encouraged by the importance of GBBR and our recent work in the area of biocatalysis, herein, we report first biocatalytic Groebke-Blackburn-Bienaymé multicomponent reaction to synthesize of Imidazo[1,2-a]pyridine derivatives using lipase enzyme [EC:1.2.2…] as biocatalyst.

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P-15

Facile synthesis of benzoxazine fused 1,2,3-triazoles via Pd-catalyzed highly selective isocyanide-insertion/cyclization/N-N bond formation cascade

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ABSTRACT: 1,2,3-Triazole fused heterocyclic compounds have attracted continuously growing attention of chemical community due to their significant applications in the various area of chemistry such as material chemistry, supramolecular, medicinal and pharmaceutical chemistry. Further, 1,2,3-triazole fused heterocyclic compounds have been found displaying a wide range of biologicalactivities such as antibacterial, anti-HIV, antitrypanosomal, antiallergic, anti-fungal, cardiovascular, antileishmanial, and chemotherapeutic activities. Among various 1,2,3-Triazole fused heterocyclic compounds, trizaoles fused benzoxazine heterocycles have been the interesting scaffolds due to their potential diuretic activities. However, a synthetic protocol to synthesize 1,2,3-triazole fused benzoxazine is very less explored. Consequently, the development of a new method to construct 1,2,3-triazole fused benzoxazine scaffolds is desirable. In this context, we have developeda new method for the synthesis of 1,2,3 triazole fused benzoxazine by the use of N-arylα (tosylhydrazine)amides with isocyanides usingPd-catalyst.

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P-16

CuI-catalyzed highly regioselective C-H functionalization of indoles using indole-3-tosylhydrazon as carbene precursors: An efficient synthesis of 3,3-bis(indolyl)methane derivatives

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Abstract: Herein, we developed a novel approach for synthesizing symmetrical as well as unsymmetrical 3,3-bis(indolyl)methane derivatives via CuI-catalyzed regioselective C-H functionalization of indole using indole-3-tosylhydrazones as carbene precursors. This process tolerates a wide range of substitutions and provides corresponding products in moderate to good yields. Further, we revealed the feasibility of this protocol in a one-pot fashion starting from indole-3-carboxyaldehyde.

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P-17

First biocatalytic aza-Michael addition of aromatic amines to enones using α-amylase in water.

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Abstract: Herein, the first example of enzyme catalyze aza-Michael addition reaction of less nucleophilic aromatic amines to enones is reported. The α-amylase from *Aspergillus oryzae* was found to efficiently catalyze this C-N bond forming reaction with a broad range of aryl (hetero) amines and enones in water as a solvent. Further, a hybrid of α-amylase with copper nanoparticle (α-amylase@CuNPs) has been prepared and used to catalyze aza-Michael addition reaction as a reusable catalyst. In particular, aza-Michael addition which leads to the formation of ß-amino carbonyl compounds has been proved most important. The ß-amino carbonyls are imperative building blocks of various biologically active compounds. Furthermore, they constitute as versatile intermediates for the synthesis of ß-lactams, aminoalcohols, and ß-aminoacids.

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P-18

Design and *In-Silico* study of novel Isatinanalogs as potential anti-HIV agents with extended activity against mutant strains

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ABSTRACT: Acquired immunodeficiency syndrome (AIDS) is an advanced stage of HIV infection. Over the past few years, the virus has been found to be resistant to most of the drugs prescribed in the Highly Active Anti-Retroviral Therapy (HAART) regimen. However, the incidences of the infection are increasing,andthus, there is a need to develop novel molecules which are active against both wild as well as mutant strains of HIV. In the current study, twelve novel Isatinanalogswere designed,andthe computational study was performedto filter out the compounds showing activity against both wild & mutant strains of HIV-1. Isatin nucleus was selected due to its broad range of pharmacological activities that have been reported by various researchers. A combination of pharmacophore based drug design andstructure based drug design approaches were used in designing the novel scaffolds. The molecules were designed as Non-Nucleoside Reverse Transcriptase inhibitors (NNRTI). The study was performed using two wild (PDBs: 1RT2 &3MEE) & two mutant strains (PDBs: 1JLA & 3MED) of HIV-1 RT enzymes. Among the twelve designed analogues, six molecules (MSG 2, MSG6, MSG7,MSG 8, MSG 9 & MSG 10) showed promising results based on docking score (MSG2: -8 TO -11.7, MSG 6: -7.1 to -13.25, MSG 7: -8.4 to -13.3, MSG 8: -5.2 to -12.9, MSG 9: -7.2 to -12.3, MSG 10: -6.4 to 11.8) and interactions with conserved amino acids like Trp 229, Phe 227, lysine 103& 101) in comparison with the standard drug Rilpivirine, Etavirine& TNK - 651.

KEYWORDS: Acquired immunodeficiency syndrome, Highly active Anti-Retroviral Therapy, Non-Nucleoside Reverse transcriptase inhibitors, Molecular Docking

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P-19

Design, synthesis and biological evaluation of 2-aminobenzimiazoles as Quorum Sensing inhibitors in *Pseudomonas aeruginosa*

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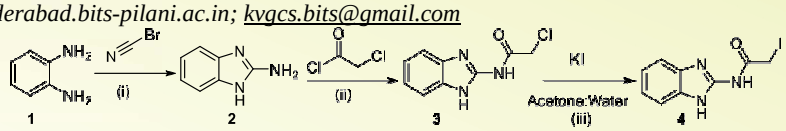
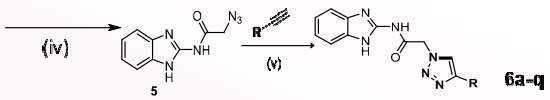


Abstract: Quorum sensing is a signaling pathway, through which bacteria regulate their phenotype, growth and population. The population density is comprehended by signaling molecules, produced by bacteria and are known as autoinducers. Inhibiting this signaling footpath through QS inhibition is one of the prospect methods to deal with bacterialinfection [1]. In our current work, seventeen 1,2,3-triazolebased2-aminobenzimdazoles are synthesized and characterized using IR, NMR, MS and elemental analysis. All the final compounds were examined for *invitro* quorum sens**i**ng inhibitory (QSI) activity against *Pseudomonas aeruginosa*. The QSI activity was determined in the LasR expressing *P. aeruginosa* MH602 reporter strain by measuring green fluorescent protein expression [2]. Among the compounds, *N*-(1*H*-benzo[*d*]imidazol-2-yl)-2-(4-(4-chlorophenyl)-1*H*-1,2,3-triazol-1-yl)acetamide (**6i)**exhibited good QSI activity with 64.99% at 250µM. *N*-(1*H*-benzo[*d*]imidazol-2-yl)-2-(4-(4-nitrophenyl)-1*H*- 1,2,3-triazol-1-yl)acetamide (**6p)** exhibited promising QSI activity 68.23, 67.10 and 63.67 % inhibition at the concentrations 62.5, 125 and 250 µM respectively. The compound **6o** displayed 64.25% QSI activity at 250 µM. In conclusion, compound **6p** is the most active QS inhibitor. The titled compounds were found less toxic at all the tested concentrations (25,50and100µM) against Human Embryonic Kidney(HEK) cell line during cytotoxicity screening studies [3]. Finally, docking study using Schrodinger Glide was also performed in order to understand the possible putative binding nature of the significantly active compound **6p** at the active site of target LasR receptor (PDB ID: 2UV0)[4].



R = alkyl/substitutedaryl/Heterocyclic

1. **Reagentsandconditions:** (i)Cyanogenbromide(1.1eq), methanol, reflux, 5min;(ii)chloroacetylchloride(1.0 eq), pyridine (2.5 eq), CH_2Cl_2, 0 °C-rt, 12h; (iii) potassium iodide (1.2 eq), acetone, 55°C, 12 h; (iv) NaN_3 (1.5 eq),DMF:Water(8:2),0°C;(v)Substituted terminal alkynes(1.4eq),$CuSO_4{\cdot}5H_2O$,(5mol%),sodiumascorbate (10 mol %), DMF:Water (8:2), rt, 6-16h.

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P-20

Eco-friendly and rapid Antimarkonikov Hydrothiolation of styrenes using Formic acid

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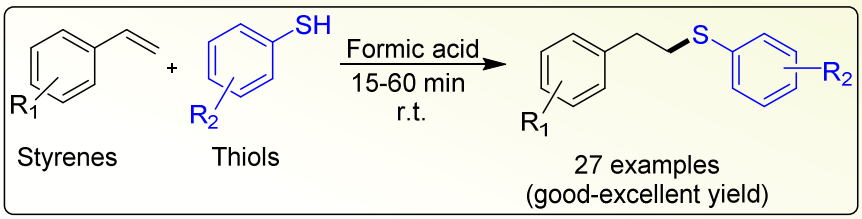
Abstract: Organosulfur compounds are valuable compound having present in numerous bioactive molecules, peptides, agrochemicals, foodstuffs, and in perfumery chemicals. These compounds are valued reagents, having importance in different organic transformations, play a key and valuable role in various areas in particular medicine and industrial processes; therefore designing new and available catalytic systems for the preparation of these compounds is one of the most important priorities among organic chemistry researches. Hence, the great importance of these molecules attracts chemists towards the development of novel, rapid and eco-friendly methodologies for the synthesis of organosulfur compounds. Herein, we have developed a novel, operationally simple, metal and solvent-free, eco-friendly and atom economically efficient methodology towards the synthesis of organosulfur compounds via the construction of C-S bond from easily available styrene derivatives with different thiophenols in presence of formic acid at room temperature. Under optimized reaction conditions, anti-markovnikov product is obtained in good to excellent yields and different functionalities are well tolerated.



Keywords: Organosulfur, Metal-free, hydrothiolation, antimarkovnikov

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P-21

Design, Synthesis and Characterizations of a Novel Series of Polyfunctionalized Fused Pyrimidines for their Biological Potential

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Abstract: Heterocycles form the basis of many therapeutic agents of which pyrimidine derivatives have played a significant role in pharmaceutical industries due it ability to exhibits a diverse array of pharmacological activities such as anticonvulsant, antibacterial, antifungal, anticancer, CNS depressant, antimalarial, antihypertensive, anti-inflammatory, analgesic, antihelmentic, antioxidant [1-3]. This broad spectrum of biochemical targets has been facilitated by the synthetic versatility of pyrimidine. There is however a lot of global health challenges with diseases such as cancer, degenerative diseases, HIV/AIDS, diabetes and drug resistant parasitic diseases of which current medicines are struggling to provide cures and hence, discovery of potential drugs candidates in these areas are urgently needed. The above forgoing challenges attracted the medicinal chemists to design and synthesize the novel therapeutic agents which are having significant therapeutic potential and accomplish the above needs. Keeping in view the above facts and importance of pyrimidine nucleus in various therapeutic targets as well as our continuous efforts to synthesize the novel lead molecules recently, we have designed, synthesized and characterized a novel series of polyfunctionalized fused pyrimidines for their biological potential. All the synthesized compounds were characterized by using various spectroscopic techniques. In this presentation, the detailed synthetic procedure, mechanisms of the reactions and characterizations of the synthesized compounds by their spectral data (^{1}H NMR, ^{13}C NMR, EIMS, UV and IR) analysis will be discussed.

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P-22

Green and efficient one-pot synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones and their anthelmintic studies

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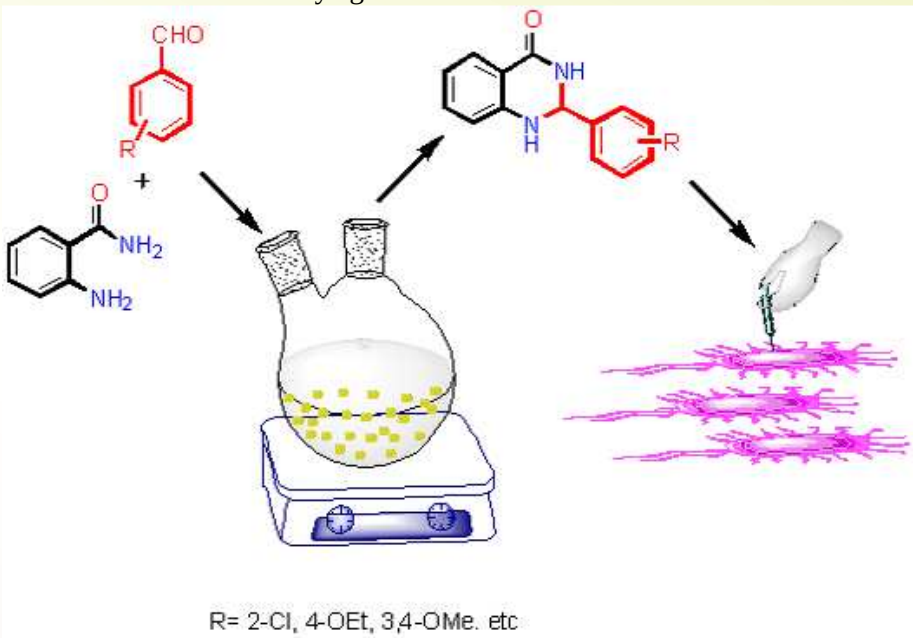
Abstract: A highly efficient and environment benign protocol for the synthesis of biologically important 2,3-dihydroquinazolin-4(1*H*)-ones derivatives has been developed by the condensation of aromatic aldehydes with anthranilamide using sulfonic acid functionalized L-Proline@Fe_3O_4 nanoparticles as a catalyst[1]. Similar to our previous reported method[2,3], this approach demonstrates several merits such as high yield, clean reaction condition, chromatography-free synthesis and easy recovery and reusability of the catalyst. In addition, the anthelmintic activities of some selective compounds were investigated and it was found that 2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one exhibited profound anthelmintic activity against two helminth models.



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P-23

Development of heterogeneous nano-catalyst and its applications for valorisation of CO/CO_2 through greener and sustainable approaches

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Abstract: Choice of mode: Poster Presentation; Date of Birth; 12/09/1992 (Shaifali), 12/01/1992 (Yamini)

The valorisation of CO/CO_2 has remained one among the foremost global challenges of the modern era as it balances the ever-increasing carbon economy. In this context, heterogeneous catalysis has been the essential tool from a long time to achieve this goal through greener and sustainable approaches from academic as well as industrial point of view.

In past few years, our group is continuously working in development of polystyrene supported transition metal nano-catalyst (TM@PS) for diverse array of organic transformations. In addition to this, our group has also demonstrated the utilisation of oxalic acid as CO/CO_2 source as an economic, easily handled and sustainable C1 source. The unique structural and morphological properties of nano-catalyst have been well exploited in valorisation of greenhouse gases (CO/CO_2) as C1 source to synthesize carbon extended industrially and pharmaceutically potent molecules. Recently, we have applied Pd@PS nano-catalyst for synthesis of substituted quinazolinones using oxalic acid as an *ex situ* C1 source [1]. Intriguingly, Pd@PS nano-catalyst in combination with oxalic acid has also been utilized for diversely substituted benzoxazinone synthesis. Furthermore, the developed strategy has also been employed for semi synthetic modification of naturally occurring himachalenes for the synthesis of bioactive pyrrolone fused benzocycloheptene analogues [2].

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P-24

Essential Oil Fraction of Oregano Abrogates *V. cholerae* Pathogenesis

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Abstract: In the age where bacterial resistance to antibiotics are increasing at an alarming rate, novel antibacterials are urgently needed to address the growing problem. Essential oils possess important volatile compounds with diverse bioactivities including antimicrobial potential. Carvacrol, an essential oil fraction of Oregano (*Origanum vulgare*) possesses wide range of bioactivities. *In-vitro* studies have demonstrated antibacterial activity of Carvacrol against pathogenic bacteria like *L. monocytogenes*, *S. typhimurium*, *E. coli* but no study has been done on *Vibrio cholerae*. Here we have studied the role of carvacrol on *V. cholerae* pathogenesis. We followed CLSI protocol to determine MIC and MBC of Carvacrol. Effect of carvacrol was investigated on mucin penetrating ability, cholera toxin (CT) production, virulence gene expression and adhesion to intestinal cell-line. In our study, MIC and MBC of Carvacrol on *V. cholerae* growth was 150 μg/ml. *V. cholerae* motility in Carvacrol treated 1.5% mucin column was 9-fold less defective. Carvacrol treated *ex-vivo* adhesion to HT-29 cell line reduced significantly by more than 100-fold at 1/3rd MIC. qRT-PCR assay revealed that carvacrol effectively repressed the transcription of different virulence genes *in vitro* at 1/4th MIC. At 1/8th MIC Carvacrol completely inhibited the biofilm formation. These results suggested that carvacrol might act as potent inhibitor of different aspects of virulence and pathogenicity of *V. cholerae*. It can be concluded that carvacrol might be added to food products at doses below the MIC value, thereby reducing the risk of adhesion and toxin production by *V. cholerae* and increasing the safety of the products.

P-25

Understanding the Prevalence and Expression of Virulence Factors harbored by Enterotoxigenic *Escherichia coli*

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Abstract: Enterotoxigenic *Escherichia coli* (ETEC)is one of the leading causes of diarrhea in infants and travelers in developing countries. Colonization factors, important for pathogenesis, are one of the main targets for ETEC vaccine development but vaccines against them had poorly performed as the prevalence of colonization factors is region-dependent. Here the presence and expression of common classical and non-classical virulence factors were studied. For the prevalence determination, PCR was employed. Quantitative RT-PCR was done to study the RNA expression of these virulence factors. Strains negative for colonization factors expression were confirmed by SDS-PAGE. Among the clinical isolates, the most prevalent toxin was *est+elt*, followed by *est* and *elt* while the pattern was reversed in the control strains. There were 29% and 40% strains negative for any classical colonization factors (CF) or non-classical virulence factors (NCVF) among the clinical and control strains, respectively. CS6 were the prevalent ones in the clinical strains as well in the control strains. For NCVF genes, *eatA* was the most prevalent among the clinical isolates and *etpA* for control. CS6 was the most expressed CF and EatA was the predominantly expressed NCVF for both clinical and control ETEC isolates. Different strains express CS6 at different levels. Not all strains expressed their respective virulence factors. Understanding the prevalent colonization factor, CS6 and its nature of expression will contribute in designing an effective vaccine against ETEC in this region of the globe. Expression pattern of CS6 also will help in examining the relatedness between the ETEC subtypes.

P-26

Pyrazolo[4,3-e][1,2,4]triazolo[1,5- c]pyrimidin-5-amine Functionalized Congeners as Bitopic Fluorescent Antagonists of A_{2A} AR

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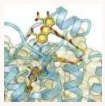
Abstract: A2A Adenosine receptor (A2A AR) antagonists are in clinical trials for the treatment of Parkinson's disease and for coadministration in cancer immunotherapy. The structures available for this receptors are useful for structure based design of adenosine receptor ligands. For further characterization of the A2A AR, various fluorescent probes have been developed over the past few years, mostly using a pyrazolopyrimidine, SCH442416. The recently reported AlexaFluor488 derivative of SCH442416 was not optimal for fluorescent binding due to its moderate hA2AAR affinity and difficulties with its green light emission. Thus, there remains a need for A2AAR antagonist fluorescent probes of higher affinity and compatibility with microscopy. A BODIPY650/655 conjugate containing a secondary amine in the linking chain was reported to have a Ki value of 15Nm for the A2AAR, but its utility was not established[1,2]. To explore the SAR of this chemical series by varying the chain length of the spacer group and the terminal fluorophore to enhance the affinity, selectivity and photophysical properties, we prepared pyrazolo[4, 3- e][1,2,4]triazolo [1,5- c]pyrimidin -5-amine antagonist of the A2AAR functionalized as amine congeners with optimal butyl spacer group, fluorescent conjugates and a sulfonate i.e. BODIPY630/ 650 derivative **11** (MRS7396, Ki: 24.6nM) and AlexaFluor488 derivative **12** (MRS7416, Ki: 30.3nM). Flow cytometry of **12** in hA2AAR-expressing HEK- 293 cells displayed saturable binding (lownonspecific) and inhibition by known A2AAR antagonists. Water-solublesulfonate **13** was a highly potent (Ki= 6.2nM) and selective A2AAR antagonist based on binding and functional assays. Docking and molecular dynamics simulations predicted interaction of distal portions of chain extended ligands with the A2AAR. The BODIPY630/650 fluorophore of **11** was buried in a hydrophobic inter helical (TM1/TM7) region, while AlexaFluor488 of **12** associated with the hydrophilic extra cellular loops. In conclusion, we have identified compound **12** and congeners a snovel high affinity antagonist probes for A2AAR drug discovery and characterization.



Molecular modeling of antagonist binding to the hA2AAR: View of the possible orientations of the fluorophore group of derivative 12

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P-27

Molecular structural Flexibility dependence of mesomorphism through ortho –Substituted nitro group"

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ABSTRACT: A novel homologous series of liquid crystals materials of schiff's base viz. RO-C_6H_4-CH=CH-COO-C_6H_4-N=CH-C_6H_4-NO_2(ortho)is synthesized and studied with a view to understanding and establishing the effect of molecular structure on liquid crystal properties and to provide novel thermotropic LC material to the scientific and technological community of research interest. The novel series consist of 12 homologues. All member of the series are enantiotropically smectogenic without exhibition of Nematogenic character. The texture of smectogenic homologoues are of the type smectic A or C. The transition temperatures were determined by an optical polarizing microscopy equipped with a heating stage. Transition curve Cr-Sm and Sm-I behave in normal manner with exhibition of odd-even effect showing phase behaviours the series. Thermal stability of smectogenic mesophase is 121.4^{0}C and mesophase length is varies between 5.0 ^{0}C to 33.^{0}C. The LC behaviour of the novel series compared with a structurally similar known series.

P-28

Design and Synthesis of Formic acid Catalyzed and Cyclised Novel Modified Route for N,7-diphenyl-7H-benzo[7,8]chromeno[2,3-d]pyrimidin-8-amine derivatives and Study of their Antimicrobial profile

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Abstract: A new series of N,7-diphenyl-7H-benzo[7,8]chromeno[2,3-d]pyrimidin-8-amine derivatives was synthesized using formic acid as catalysed and solvent. The structures of the new derivatives were confirmed by the spectral data and elemental analyses. More over Anti-microbial and Anti-fungal activities has been carryout using S. aureus, S.pyogenes, E.coli, P.aeruginosa, C.albicans, A.niger and drugs Nystatin, Greseofulvin, Ciprofloxacin, Chloramphenicol for all new novel compounds.

P-29

A rapid one-pot Synthesis and Biological Evaluation of Novel 1,2,4-Triazolo[1,5-a] pyrimidines

V. H. Shah, M. H. Chauhan

Abstract: The synthesis of ten novel 1,2,4-Triazolo[1,5-*a*]-pyrimidine derivatives have been undertaken by involving Biginelli type three components reaction of 1-phenyl-3-aryl-1H-pyrazole-4-carbaldehydes, 3-amino-1,2,4-triazole and ethyl acetoacetate in DMF. The constitution of all the compounds have been established by extensive use of analytical tools *viz*; IR, FT-IR, ^{1}H-NMR, ^{13}C-NMR, Mass spectra studies and elemental analyses. The antimicrobial activity *against S. aureus* MTCC-96 (gram-positive), *E. Coli* MTCC-443 (gram-negative) and antifungal activity against *A. niger* MTCC-282 and C. *albicans* MTCC-227 at different concentrations using micro-dilution broth method according to NCCLS standards. The antimicrobial activity was compared with Ampicillin, Chloramphenicol, Ciprofloxacin, Norfloxacin, Nystatin and Greseofulvin as standard drugs at same different concentration.The antimicrobial activity was measured in the zone of inhibition in m.m.The compounds such as A-2, A-4, A-5, A-6, A-8, A-9, A-10 showed moderate antibacterial activity against *stapsylococcusaureus* (gram positive) at the concentration of 250, 100, 250, 200, 250, 250, 250 µg/ml while A-3, A-6 showed remarkable antibacterial activity against *Streptococcuspyogenes* (gram positive) at the concentration of 100 µg/ml. Moreover,the compounds A-3, A-9, found to be potent against *Escherichia coli* (gram negative) at the concentration of 62.5, 62.5 (µg/ml) and against *Pseudomonas aeruginosa* (gram negative) with the concentration of 100 µg/ml.

P-30

Synthesis and Biological evaluation of Highly Functionalized Derivatives of Acredonyl-Pyrimidines via Chalcone formation

V. H. Shah, H. P. Parekh

Abstract: In this article, the synthesis of heterocyclic 2 **– (2,3- dihydro –2-oxo-6-aryl-4-yl)-acridin-9(10H)-ones (HPV 1–HPV 10)** have been undertaken by reaction of 2-(3-aryl-4-yl) acridin-9(10H)-ons (Chalcones) (III1- III10) with urea in presence of catalyst KOH under reflux 4 hr. The synthesis of **2-(3-aryl-4-yl)-acridin-9-(10H)-one (Chalcones)(III 1- III 10)** have been carried out by the condensation of 2-acetylacridine-9(10H)-one (II) with aromatic aldehydes in presence of ethenolic potassium hydroxide. 2-Acetylacridin-9(10H)-one (II) was prepared by the cyclisation of 2-(4 acetylphenylamino)-benzoic acid (I) in poly phosphoric acid (PPA) as phase transfer catalyst. 2-(4 acetylphenylamino)-benzoic (I) further synthesized by the reaction of 2-chloro benzoic acid with 4-amine Acetophenone in presence of Cu, DMF and K_2CO_3 as a weak base at 110-120 ^{0}C for 3 hrs involving Ulmman reaction as per reaction scheme-1. The constitution of all synthesized compounds (HPV – I to HPV -10) has been elucidated by Ft- IR, 1H- NMR, Mass spectral data and elemental analyses. The Newly synthesized compounds (HPV–I to HPV-10) have screened for antimicrobial biological activity viz. antibacterial and antifungal activity. All compounds showed good to moderated activity against gram positive and gram-negative bacteria species as compared to standard drugs and moderate activity against fungal species.

P-31

Trifluoroacetic Acid Catalyst for Self-Condensation of Acetophenones in Presence of Selenium Dioxide: Enantioselective Synthesis of Fused [1,3]dioxolo[4,5-d][1,3]dioxoles.

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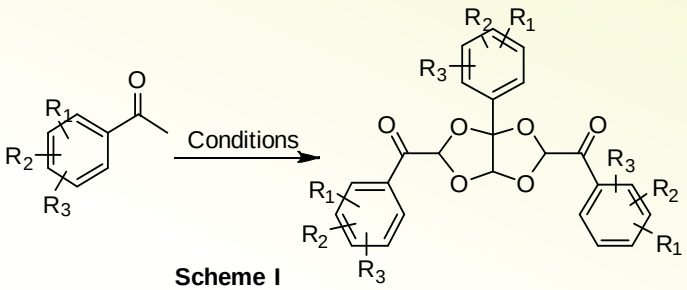
Abstract: Heterocyclic compounds constitute the largest family in organic compounds and are common scaffold found in natural products. They are also common motifs in synthetic compounds which possessed biological activities. As a consequence of this the synthesis of heterocyclic compounds is still a promising challenge in the field of organic chemistry. In particular, heterocyclic compounds with oxygen hetero atom generates a wide scope because of its high natural occurrence abundance and of their presence in biological active compounds. As part of our continuing effort to develop newer synthetic methodologies in organic synthesis through the intermediary selenium dioxide[1, 2] we wish to report here a single step method for enantioselective self-condensation reaction of acetophenones in presence of SeO_2 catalysed by trifluoroacetic acid where three molecules of acetophenones condenses efficiently to deliver substituted [1,3]dioxolo[4,5-*d*][1,3]dioxoles in moderate to high enantiomeric excess (Scheme I).



Scheme I

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P-32

Synthesis and Molecular folding studies in Pyranone Carboxamide through 1, 2-diamino benzene bridge

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Abstract: The destruction of the immune system by the virus results in opportunistic infection, as well as an increased risk of autoimmune disease. It was observed that drug resistant viruses and side effects demand the requirement of development of new scaffolds. Herein, we report discovery of new scaffold based on pyranone-carboxamide analogue as promising anti-HCV agents as well as almost all types of pharmacological activities such as anti-inflammatory, anti-psychotic, anti-obesity etc. As our supramolecular scaffolds possess multiple well defined covalent or non-covalent binding sites for target molecular units assemble into a structure whose morphology and size regime basically reflect supramolecule. Hereby, we synthesize a pyranone-carboxamide through the pyranone based acid using oxalylchloride and further ArSn1-substitution of SMe was done by morpholine.

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P-33

Bromination of *α,β*-Unsaturated ketones using *N*-Bromosuccinimide in the presence of Selenium Dioxide and *p*-Toluene sulfonic acid: An efficient protocol for the synthesis of (*E*)-1-bromo-4-arylbut-3-en-2-one.

Tyrchain Mitre Lipon, Ibakyntiew D. Marpna, Bekington Myrboh

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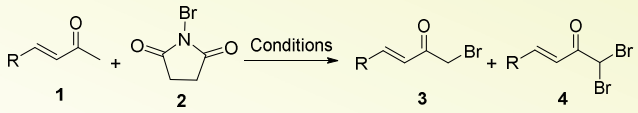
Abstract: A highly efficient method has been developed for the synthesis of variously funtuntionlized *α,β*-unsaturated *α'*-haloketones using *N*-bromosuccinimide mediated by selenium dioxide in presence of *p*-toluene sulfonic acid as a catalyst. The present method is regioselective, employing easily available and affordable starting reagents. The short reaction time, simple workup and good yield of the products make this protocol an attractive alternative for the synthesis of *α,β*-unsaturated 1-bromo-2-ones (**3**), and it is interesting to note that some reactions yielded the dibromo product **(4**) as a minor component (**Scheme 1).**



Scheme 1

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FACICL SYNTHESIS OF SOME 3-METHYL-1, 4 –DIHYDROPYRANO [2, 3-C] PYRAZOLE DERIVATIVES AND THEIR ANTICANCER ACTIVITY

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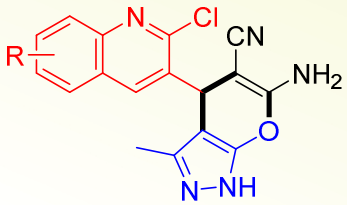
Abstract: Nitrogen congaing heterocycles have prominent feature in the field of cancer drugs there by. More over amino cyano group has also process important treatment for drug metabolism due to the free-NH2 group. From the above activity effect of cyano group as well as presence of nitrogen in five and six membered ring system. We have synthesis fused Pyrazole Pyran derivative bearing quinolone nucleus. All the synthesized compounds were well characterized by various spectroscopic methods like IR, Mass and NMR. The decline of the synthesis product for anticancer amine was carried out by using PASS-online and further evaluation for the anticancer activity. The results of compound shown that synthesized compounds have been evaluated for their in vitro anticancer activity against NCI-60 cancer cell lines.The findings revealed that one synthesized compound exhibited significant anticancer activities against SR (leukemia) RPMI-8286 and Colon cancer cell lines.



(**DSS**-1a to 1f)

DSS-1a, R=6,7 diCH_3; **DSS-1b**, R=-H; **DSS-1c**, R=6-Cl; **DSS-1d**, R=6-OCH3; **DSS-1e**, R=6,8-diCl; **DSS-1f**, R=6-Br

Keywords: Green chemistry, 2-Chloroquinoline-3-carbaldehyde, Pyrano[2,3-c]pyrazole, Anticancer agents, Leukemia cancer and Colon cancer

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ONE POT SYNTHESIS OF SOME 3-METHYL-1, 4 –DIHYDROPYRANO [2,3-C]PYRAZOLE DERIVATIVES AND ITS ANTICANCER SCREENING

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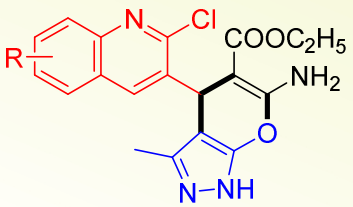
Abstract: Literature survey reveals that pyran derivatives possess very prominent position in medical field due to their wide range of biological activities. More over pyrazole and quinoline also have been found important position in the field of medical chemistry. From the above finding we have clubbed 2-chloroquinoline-3-carbaldehyde, ethyl 2- cynoacetate and pyrano [2,3-*c*]pyrazole to enhance their impotence in this field. All some compounds have been selected for anticancer basis of pass online. The findings revealed that one of the synthesized compounds exhibited significant anticancer activities against leukemia, specifically **DSS-3f** which shown the highest activity among the tested compounds against SR (renal) cancer cell lines.



(**DSS**-3a to 3f)

DSS-3a, R=6,7 diCH_3; **DSS-3b**, R=-H; **DSS-3c**, R=6-Cl; **DSS-3d**, R=6-OCH3; **DSS-3e**, R=6,8-diCl; **DSS-3f**, R=6-Br

Keywords: Green chemistry, 2-Chloroquinoline-3-carbaldehyde, Pyrano [2,3-c]pyrazole, Anticancer agents, Renal cancer

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P-36

GREEN APROACH FOR SYNTHESIS OF 3-METHYL-1,4 –DIHYDROPYRANO [2,3-C]PYRAZOLE DERIVATIVES AS ANTICANCER AGENTS

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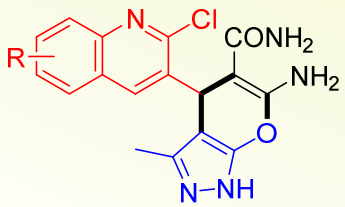
Abstract: We have clubbed pyrazolopyran with quinoline nucleus by using green one pot synthesis approach. All the synthesized compounds were obtained enough pure without any purification in good yield. All the synthesized compounds were well characterized by various spectroscopic methods like IR, Mass and NMR. Some selected compounds have been evaluated against 60- cancer cell line to check their potency. The findings revealed that some of the synthesized compounds exhibited significant anticancer activities against leukemia, specifically **DSS-2d** and **DSS-2a**which shown the highest activity among the tested compounds against SR (leukemia) HL-60(TB) and K-562 cancer cell lines.



(**DSS**-2a to 2f)

DSS-2a, R=6,7 diCH_3; **DSS-2b**, R=-H; **DSS-2c**, R=6-Cl; **DSS-2d**, R=6-OCH3; **DSS-2e**, R=6,8-diCl; **DSS-2f**, R=6-Br

Keywords: Green chemistry, 2-Chloroquinoline-3-carbaldehyde, Pyrano [2, 3-c] pyrazole, Anticancer agents, Leukemia cancer

Reference:

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P-37

Isolation of chemical markers and their quantification for quality control of *Polygonatum verticillatum*

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Abstract: *Polygonatum verticillatum* [L.] All. is an ancient medicinal plant among astavarga of Ayurveda. The plant has abundant demand in the global market, its limited chemistry, confusion in vernacular names and lack of reliable analytical method provides the liberty to user for substitution and adulteration. Virk et al. [1] Quality control is very crucial in rendering traditional medicinal into evidence-based modern therapies. Neelam et al. [2]FDA guidance recommends the quality control tests for the Botanical Drug which should cover chemical identification by spectroscopic techniques HPLC, UPLC, HPTLC, and GC LC-MS. In present, no analytical method is available for the quality control of Polygonatum and its value-added products. Hence in this study isolation of chemical markers and development of a novel and efficient UHPLC method was focused. Markers includes a flavonol glycoside rutin (1), two flavonol quercetin (2) and kaempherol (3), and three homoisoflavonoids 5,7-dihydroxy-3-(2-hydroxy-4-methoxybenzyl)-chroman-4-one (4), 5,7–dihydroxy-3-(2-hydroxy-4-methoxybenzyl)-8-methylchroman-4-one (5) and 5,7–dihydroxy-3-(4-methoxybenzyl)-8-methylchroman-4-one (6). The separation was achieved within nine minutes on C-18 column using gradient elution of acetonitrile and water containing 0.1% formic acid. The method was validated for its linearity, precision (inter and intraday), accuracy, limits of detection and quantification as per international Council for Harmonisation guidelines (ICH). The validated method was applied for the simultaneous quantification of compounds 1-6 in samples of *P. verticillatum*. Developed method will be helpful to assess the quality of P. verticillatum raw material and their derived products.

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P-38

QUINOLONE ESTERTAGGED THIAZOLESUBSTITUTED TACRINE ANALOGS AS DUAL BONDING SITE ACETYLCHOLINESTERASE INHIBITORS FOR ALZHEIMERS TREATMENT

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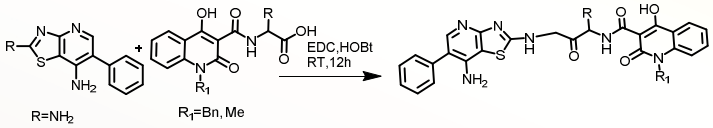
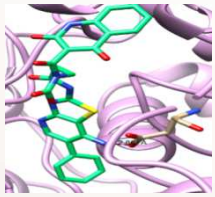
Abstract: Among all the neurodegenerative diseases (NDs), Alzheimer's disease (AD) has now become a big medical problem, especially in the countries where the population's age is increasing. The progress of AD involves a severe loss in memory and cognition leading to behavioral changes, depression, and an eventual death and hence requires immediate therapeutic intervention. AD is broadly recognized as a multidirectional disease, and the multiple origin of the pathology suggests that a key strategy for the preparation of new drugs could be found in the so-called "multi-target ligands"approach [1].One major strategy for the development of new therapeutics relates to the enhancement of cholinergic system through anticholinesterase inhibitors and has generated a lot of attention culminating in the development of different marketed drugs.Tacrine (1,2,3,4-tetrahydro-9-aminoacridine; THA) is an active acetylcholinesterase inhibitor administered to thousands of patients for the treatment of Alzheimer's disease (AD) [2]. The clinical use of tacrine, as a reversible AChEI and Butyrylcholinesterase (BuChE) inhibitor, was discontinued due to its hepatotoxicity. However, tacrine has been selected as the ideal active fragment because of its simple structure, clear activity and its superiority in structural modifications and thus it could be introduced in modified form into the overall molecular skeleton of multitarget directed anti Alzheimer's agent. In our present work, we have rationally designed such agents based on their *in-silico*studies. During *in-silico*studies we got some interesting results showing high docking score for the compounds in which quinolone is attached with tacrine analogue through thiazole ring side. These compounds were able to penetrate deep inside the gorge of acetylcholinesterase enzyme which encouraged us to move towards the synthesis of such compounds.Based on docking studies and our experience in synthesis, we plan topreparean array of thiazole substituted quinolone ester tagged tacrine analogs with a change in linking position in tacrinethus leading tomuch lower toxicity than the standard drug donepezil.The scheme for the synthesis of desired compounds is as given below.





LIGAND	MOL FORMULA	M.W.	Qlog Po/w	H-B D	H-B A	fMET	LD50 (mg/kg)	DOCKING SCORE
Donepezil	$C_{24}H_{29}NO_3$	379.498	4.292	0	5	6	505	-10.988
PS-06	$C_{27}H_{32}N_4SO_4$	520.605	3.5	3	8	5	10,000	-8.388
PS-09	$C_{25}H_{28}N_4SO_4$	464.498	2.359	3	8	5	2100	-8.296
PS-11	$C_{28}H_{33}SN_3O_3$	507.523	1.168	3	10	6	600	-8.418
PS-12	$C_{28}H_{33}N_3SO_3$	507.523	1.307	3	10	7	505	-9.196
PS-37	$C_{28}H_{32}N_4SO_4$	532.644	4.371	2	9	7	3540	-8.047
PS-44	$C_{32}H_{30}N_2O_4$	502.572	5.182	2	6	6	5000	-9.208

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P-39

Isolation of starch from turmeric residues and its characterization

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Abstract: The present work was aimed to evaluate the different properties of turmeric starch. Turmeric starch was isolated from residues of *Curcuma longa* L. (Zingiberaceae). In this article, we established an easy and straightforward method of isolation of starch from the wastes of turmeric. Along with physical, physio-chemical characteristics were studied like, microscopical, SEM analysis Dhanalakshmi Kuttigounder et al [1], size and shape, particle size distribution (2-32 µm), molecular weight determination by gel permeation chromatography Graham Cleaver et al **[**2**]** (GPC) (372267g/mole), pH of turmeric starch solution **[**3**]** (5.6), specific surface area by BET analysis Ricco A J et al **[**4**]** (0.69 m^2/gm), moisture content Medcalf D G et al **[**5**]** (15%), true density USP **[**6**]** (0.568 g/cm3), Iron content USP **[**7**]** (less than 10 ppm), viscosity of starch solution (1209 cP), and gelatinization temperature (80°C) etc. Remarkably turmeric starch has shown consistency and temperature-dependent gelatinization property AACC Intl **[**8**]** within 20 min at 80°C. The main aims of this work to increase the applications of starches in industries by analyzing different sources of starches.

Key words: Turmeric starch, Gel permeation chromatography, Viscosity, *Curcuma longa*.

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P-40

Spectrophotometric determination of hydrophilic Crystal violet dye with Spices derivative analogue Nutraceutical Chilli seed spent

Chaya G and Bibi Ahmadi Khatoon

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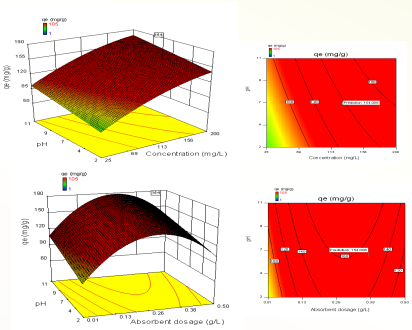
Abstract: The present research study approach towards adsorption an efficacious remedy for hydrophilic crystal violet dye with endemic spices analogue Nutraceutical chilli seed spent. The study identified the pattern of adsorption assay which precede various factors like effect of temperature, Initial dye concentration, pH, kinetics which confer an effective adsorption responsive surface treatment dependent on dosage form entities has been used extensively to investigate adsorbate – adsorbent molecules surface interaction. The data experimental value of the adsorption capacity, q_e was 70 mg/g. The Size determination of Nutraceutical Chilli seed spent polydispersity index shows 0.266 with z-average 247.9 and intercept 0.873. The characterization were carried out by SEM analysis reveals adhesion of dyes on their porous structural surfaces and FTIR analysis to interpret the functionalgroups on adsorption sites which favors adsorption on surfaces favorable and effective in deposition of Crystal violet dye.

Keywords: Spectrophotometric assay,Spices derivative analogue Nutraceutical Chilli seed,Precursor



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P-41

Characterization of novel Isoxazolone(4-Arylmethylidene-3-substituted-Isoxazol-5(4H)-ones) derivatives as anticancer compounds using *Insilico* methods

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ABSTRACT: Cancer is a disease of striking significance in the world today. The identification of novel structures that can be potentially useful in designing new, potent, selective and less toxic anticancer agents is a major challenge in medicinal chemistry [1]. Isoxazolone, oxygen–hydrogen-containing five membered heterocyclic compounds show excellent biological activities. In the present study we have demonstrated a computational and experimental approach to identify the anticancer propertiesof newly synthesized novelisoxazole derivatives. Such integration of computational and experimental strategies has been of great value in the identification and development of novel promising compounds. Twenty different derivatives of 4-arylmethylidene-3-substituted-isoxazol-5(4H)-ones were synthesized by green chemistry method [2].These compounds were screened for ADME analysis using SwissADME. 27 different proteins interacting with routine anticancer drugs were selected from NCI database and all 20 compounds and their conformersdocked against these proteins using PyRx [3].All compounds were showing good fitting and caused favorable contacts with proteins ABL kinase and tubulin b. The DisGenNETdatabase revealed that ABL kinase and tubulin b control various oncogenic signaling pathways, and also associated with different cancers, metastasis and overall prognosis.The computational data obtained was supported by *in vitro* cytotoxic assay against two cell lines Caco-2 and MCF-7. These compounds were investigated for their effect on mitosis using *Alium sativum* roots.In was observed from *in vitro* data that some compounds were showing positive results in correlation with*insilico* analysis. In conclusion, a series of 4-arylmethylidene-3-substituted-isoxazol-5(4H)-one derivatives have potential to become lead molecules as anticancer drugs.

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P-42

Development of naturally inspired (E)-3-(4-hydroxy-3-methoxyphenyl)-1-(4-phenylpiperazin-1-yl)prop-2-en-1-one derivatives as multifunctional agents for the treatment of Alzheimer's disease

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[#]*DoB 27.08.1994*

ABSTRACT: Alzheimer's disease (AD) is a multifactorial progressive neurodegenerative brain disorder characterized by gradual loss in memory and normal functions. It is the sixth-leading cause of death in the United States. In India approximately 4.1 million people are suffering from AD. Currently available treatments for AD in the market provide only symptomatic relief for the initial short period of time. Acetyl and Butyrylcholinesterase(AChE & BChE) play a key role in AD. Natural products including ferulic acid (FA) have shown promising anti-AD property due to potent inherent antioxidant potential. However, weak interaction with the key target enzymes (AChE & BChE), and selectivity for the target are major limitations associated with natural drugs including FA. To overcome these limitations and develop the druggable natural product based therapy for AD, we have carried out SAR studies on FA. The enzyme inhibitions and kinetic studies identified compound 10b as one of the lead molecule with preferential acetylcholine esterase inhibition properties (AChE:IC50= 9.91±0.07μM) compared to the parent molecule ferulic acid (% inhibition at 20μM, AChE= 15.194±0.59μM;).10b was found to be an efficacious antioxidant in DPPH assay (IC_{50} =61.98±0.μM). The detail biological and computational studies are ongoing and will be presented.

P-43

Synthetic and mechanistic studies on the organo-nanocatalyzed synthesis of Spirooxindole derivatives under ultrasonication and its activity against *raillietina sp* and *syphaciaobvelata*

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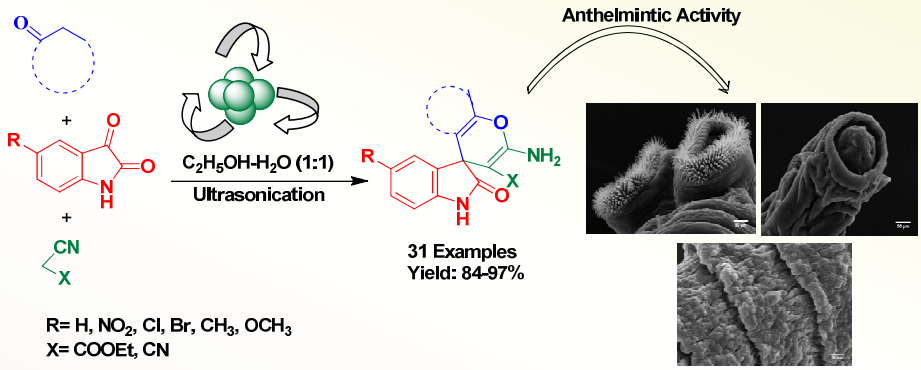
ABSTRACT: A new class of organo-nanocatalysts was fabricated by encapsulating magnetic Fe_2O_3@SiO_2 nanoparticles with thiamine hydrochloride. The prepared catalyst was characterized by various analytical techniques *viz.*, FT-IR, TGA, TEM, SEM, EDX, Powder XRD and VSM and its catalytic activity was investigated for the synthesis of spirooxindole derivatives. Utilizing the ferromagnetic nature of core Fe_2O_3 nanoparticles, the encapsulated catalyst could be easily retrieved from the reaction mixture after completion of the reaction by using an external magnet. The catalyst was reused up to six runs with remarkable catalytic activity. The main advantages of this synthetic approach lie in its operational simplicity, cost effectiveness, higher yields, easy catalyst recyclability and reusability, eco-friendly procedures and shorter reaction times. Mechanistic studies for the organic transformations were also carried out to determine. The catalytic role of thiamine hydrochloride using a computational method viz. DFT: B3LYP. Also, the anthelminthic assay of the synthesized spirooxindoles was evaluated against *raillietina sp* and *syphaciaobvelata* and the results showed profound anthelmintic activities.



Graphical Abstract

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P-44

N-Heteroarylation and Solvent-Switched Acetoxylation and Alkoxylation in Mannich Bases of Imidazopyridines*via* PIDA-Mediated 1,2-*Ipso*-Migration

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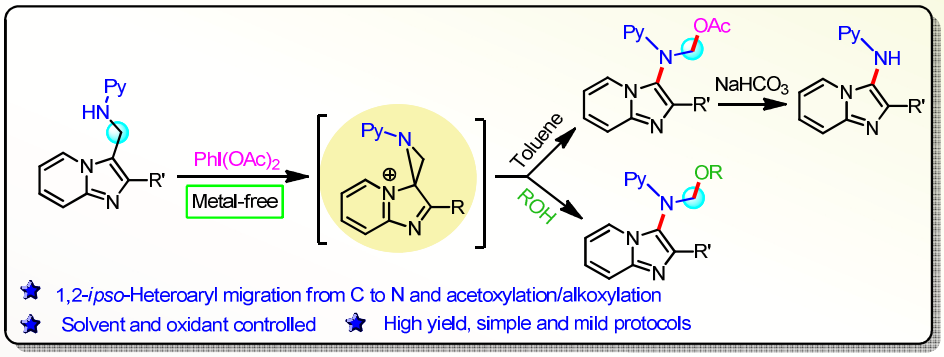
ABSTRACT: *ipso*-Migration is an emerging and attractive approach to synthesize a variety of spirocyclic and complex molecules and have been demonstrated as an efficient tool in the synthesis of highly functionalized heterocycles.[1]Intramolecular *ipso*-migration of arenes or heteroarenes *via* C-C bond cleavage is an interesting area of research in synthetic organic chemistry.[2] Carbon to carbon migration of arenes and heteroarenes has been explored in great details,[3] but migration from carbon to nitrogen of arene or heteroarene ring is rarely explored.

On the other hand, hypervalent iodine(III) reagents have been considered as effective reagent for oxidative rearrangements due to their electrophilicity and good leaving group tendency as well as their environmentally friendly behavior.[4] These reagents have been successfully employed for the oxidative rearrangement of arene ring through ring expansion, ring contraction, or arene or heteroarene migration.[5] We report a novel hypervalent iodine(III) reagent-mediated oxidative rearrangement in Mannich bases derived from imidazo[1,2-*a*]pyridines, 2-aminopyridines and formaldehyde. It is proposed that the reaction proceeds through heteroaryl 1,2-*ipso*-migration *via* the formation of aziridine intermediate. The method has been utilized for the synthesis of various 3-aminoimidazo[1,2-*a*]pyridine derivatives. A solvent-switched functionalization of the product was observed. Details will be presented in the poster.



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P-45

A Novel One-pot Co(II)-catalyzed Synthesis of Imidazopyridine Derivatives

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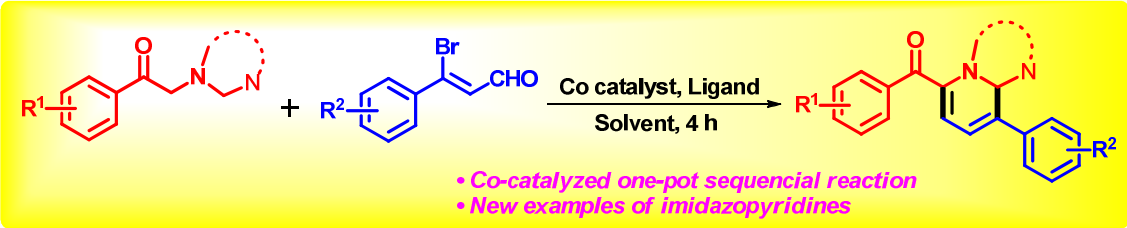
ABSTRACT: Imidazoheterocycles are privileged *N*-heterocycles and have been reported to exhibit a broad range of biological and pharmaceutical properties. Mostly,imidazo[1,2-*a*]pyridine are found in a number of commercially available drugs such as necopidem, saripidem and GSK812397 for anxioselective activity.[1] We became interested in developmentof new protocols for the synthesis of these fused aza-heterocycles because of enormous biological and pharmaceutical chemistry activities.[2]On the other hand, transition metal–catalyzed cross coupling and C-H activation/ functionalization has emerged as a powerful tool for the construction of complex structural molecules in organic synthesis.The selectivity and atom economy feature make this strategy more environment friendly as compared to traditional cross coupling reactions. The construction of targeted C–C bond to access fused aza-heterocycles by using simple commercial starting materials is still a challenging task for organic chemists.[3] Herein, we report an efficient and convenient one-pot sequential strategy for synthesis of polysubstituted imidazopyridine (Scheme 1). The reaction involves tandem Knoevenagel type condensation of active methylene azoles and 3-bromocinnamaldehydesfollowed by Co(II)-catalyzed intramolecular oxidative C-C coupling reaction.This protocol opens a new route to synthesize functionalized imidazopyridine derivatives. Details of the developed protocol will be presented.



Scheme 1: Co(II)-catalyzed synthesis of imidazopyridines

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P-46

Effect of Short-term westernized (HFFD) on glucose homeostasis, Hippocampal insulin signaling, and related cognitive and recognition memory function.

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Abstract: Excessive consumption of high-fatfructose diet (HFFD) is associated with the development of systemic insulin resistance (InsRes) and further progression into type-2 diabetes (T2DM). InsRes induced hippocampal insulin signaling has serious consequence on hampered sensorimotor, cognitive performance and long term potentiation accompined to neuronal cell death in hippocampus.However, short-term HFFD/(STZ) mediated hippocampal InsRes and related neurobehavioral alterations in adoloscents has not been reported. Therefore, we investigated a one-week HFFD model to augment the state of InsRes along with a single sub-diabetogenic dose of STZ (45 mg/kg i.p) to produced a hampered hippocampal insulin signaling associated with frank hyperglycemia and other biochemical and neurobehavioral alterations in young rats.To achieve this, male wistarrats of age (8-10 weeks) and weight 80–120 gwere divided into two main groups: (1) fed withcommercial standardnormalfat diet (NFD: 6.5 % kcal fat) and (2) fed an in- house prepared high-fat diet [HFFD: 58 % kcal fat]and 20% high-fructose corn syrup in the distilled water.Our results showed that anincrease in calorie intake, water intake, body weight and blood glucose levels. Further, an increase in fasting serum insulin and Homeostasis Model Assessment-index (HOMA-I) and OGTT was observed. Whereas, a down-regulation of hippocampal insulin receptors (IR) and P-Akt which plays a principal role in insulin resistance in hippocampus was evident, indicating biochemical alterations in hippocampus resulting in cognitive dysfunction and hypolocomotion.

Keywords: High fat fructose diet; Hippocampal Insulin Signalling; Cognition; GLUT 4; BDNF; HOMA-I

P-47

Ruthenium Catalyzed [4+1] Annulation of 1-Arylindazolone with acrylates: An Access to indazoloindazolone derivatives

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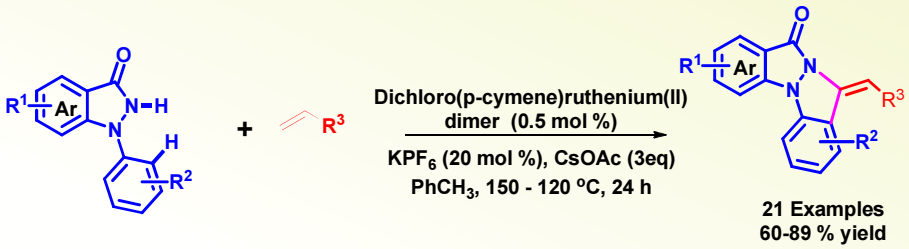
ABSTRACT: The diazaheterocycle indazolone shows important biological activities such as anti-cataract, antitumor, antibacterial, anti-inflammatory,antiasthmatic, antipsychotic, antifertility, antihyperlipidemic, antihyperglycemic,antagonist, antichagasic, activities.[1] Also indazolone scafold containingderivatives has been used in the polymers, plastics, sensors, gelators, LEDs *etc*.[2]In the past few years various groups explored the synthetic strategies of fused or functionalized indazolones[3]*via* transition metal catalysis by using diazocarbonyls[4] and alkynes[5] as coupling partners. In spite of previous synthetic wisdom collated, developing efficient synthetic strategies for the construction of fused indazoles are still of great intrest and in demand.



An efficient one-potRuthenium-catalyzed strategy for the synthesis of fusedindazoloindazolones was developed by [4+1] annulation of 1-arylindazolones and acrylates*via* sequential C-H activation/alkene insertion/cyclization in a tandem fashion. The protocol showcased excellent tolerance towards electron-withdrawing as well as electron-donating functional groups on 1-arylindazolone.

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P-48

Facile Synthesis of *N*-Arylquinolinoporphyrins*via*PIFA-PromotedOxidative Cyclization of β-Aminotetraarylporphyrins

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ABSTRACT: Tetrapyrrolic macrocycles like porphyrins play an important role in various fields such as catalysis,supramolecular chemistry,biomimetic models for photosynthesis,electronic materialsand medicinal chemistry [1].Also, they have enormous potential for their usefulness as supramolecular assemblies, artificial light-harvesting, catalysis, sensing, nonlinear optics and drugs [2].The chemical transformation of porphyrins into new derivatives with improved features that may turn them into possible candidates for different applications. Among the available synthetic tools for porphyrin functionalization,fusion of aromatic rings with the porphyrin nucleusis the most obvious way to extend the molecule [3].Physicochemical and redox properties of porphyrinoids also depend on nature and number of substituent's present at core macrocycle [4].The properties of porphyrinoids could be tuned by introducing substituents selectively either at β or *meso*-positions. The π-conjugation through extension, fusion, and dimerization may also alter the properties of porphyrinoids. Particularly, fused porphyrins embedded with heteroatom are one of the most promising porphyrinoids in the area of molecular electronics and nanotechnology.π-Extended porphyrinoids have been utilized in the fields of solar energy harvesting and photodynamic therapy [5]. In the present work, avariety of *N*-arylquinolinoporphyrins were easily synthesizedinvolving PIFA-mediated intramolecular oxidative cyclization and Cu-catalyzed *N*-arylation of *in-situ* generatedenamino porphyrins.*In-situ* generated iodoarenes from the PIFA-promoted intramolecular cyclization of readily accessible β-aminotetraporphyrinswere effectively utilized in the formation of carbon-nitrogen to accessvarious*N*-arylquinolinoporphyrins.Prepared arylquinolinoporphyrins were adequately characterized by NMR (^{1}H &^{13}C) and Mass spectrometry spectral data, and some of the heteroaromatic porphyrins displayeda significant shift in absorption and emission bands.

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P-49

Indolyl-α-keto-1,3,4-oxadiazoles as Tubulin Interacting Agents

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ABSTRACT: Microtubule cytoskeleton are composed of α and β tubulin hetero dimmers[1].They play key role in numerous biological functions such as intracellular transport of cellular components during interphase, developing the mitotic spindle throughout the cell division as well as maintaining the cell motility and cell morphology. For this reason, chemical agents that interfere with microtubule cytoskeleton functions are found to have broad spectrum of anticancer activity[2].In the past few years; indole has been introduced as a privileged moiety in the field of drug discovery and development [3].Among the indole analogues, aroylindoles, arylthioindoles, indibulin, 2-aryl-4-benzoylimidazoles,diarylindoles, have beenreported to show significant inhibition of tubulin assembly [4].In order to identify some potent indole-based anticancer agents, recently we identified various indolylazoles with enhanced cytotoxicity; for example, indolylisoxazolines,bis(indolyl)ketohydrazide-hydrazones, 5-(2'-indolyl)-thiazoles, 2-arylamino-4-(3'-indolyl)-thiazole[5].In continuation to discover potent cytotoxic indoles, in the present work we have designed and synthesized novel indolyl-α-keto-1,3,4-oxadiazoles by using molecular iodine mediated oxidative cyclization of acylhydrazones.Preparedindolyl-keto-oxadiazoles were well characterized by using various spectroscopic techniques including IR, NMR and HRMS. Anticancer activities of the compounds were screened *in-vitro*against various cancer cell lines such as human lymphoblast (U937), leukemia (Jurkat& SB) and human breast (BT474).Someof the compounds showed potent *in-vitro* anti-proliferative activity against panel of cell lines with IC_{50} values in low micromolar range.Also, molecular docking studies of the most potent compound (IC_{50}= 10.66µM) suggested a potential binding mode at the colchicine binding site.

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P-50

DEVELOPMENT AND VALIDATION OF A STABILITY INDICATING RP-HPLC METHOD FOR SELEXIPAG

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ABSTRACT: Selexipag is developed for the treatment of pulmonary arterial hypertension (PAH, WHO Group I) to delay disease progression and reduce the risk of hospitalization for PAH. An attempt was to develop and validate a stability indicating RP-HPLC method for the quantification of Selexipag in bulk form. The developed method was validated according to International Conference on Harmonization guideline with respect to limit of detection (LOD) and limit of quantification (LOQ), linearity and range, specificity and system suitability. For this, an isocratic condition of mobile phase comprising buffer and acetonitrile at a flow rate of 1.0 mL/ minute over Inertsil ODS-3 C18 Column (250 x4.6mm,5 µm) column at 28°C temperature was maintained. The detection was done using a PDA detector at 303 nm. The method was found to be within the limit of correlation coefficient (R2 ≥ 0.995). The percent recovery was found within the acceptance limit of 98.0% to 102.0% . Stress degradation studies including photolytic degradation, oxidative degradation, acid degradation, base degradation and thermal degradation were carried out. Method has been successfully applied for assay of Selexipag from marketed formulation.
Keywords: Selexipag, ICH guidelines, RP-HPLC, Validation

P-51

TiO_2 as reusable catalyst for synthesis of 5-arylidine-2,4-thiazolidinediones under solvent free conditions.

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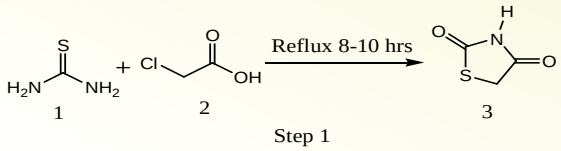
Abstract: The 2,4-thiazolidinedione derivatives are important for its diverse biological properties such as antibacterial and antifungal, antiviral, antitumor and antidiabetic activities.[1, 2] Synthetic development of biologically important derivatives is necessary. Many attempts have been carried out such as piperidinium benzoate [3], baker's yeast, and ionic liquids [4] etc. But these are not suitable to the point of environment. Therefore, this condensation reaction required further improved. Metal nanoparticles particularly, based on TiO_2 are inexpensive, easy to synthesize and effectively used for organic synthesis reaction.

A efficient solvent-free method for synthesis of 5-arylidine 2,4-thiazolidinediones by the knoevenagel condensation of aromatic aldehydes with 2,4-thiazolidinedione using TiO_2 as a recyclable heterogeneous catalyst is described. In present study satisfactory results are obtained with excellent yield of products, simple procedure and short reaction time.



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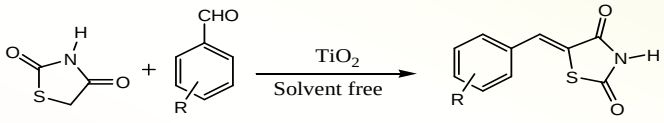
Step 1



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Step 2

Keywords: TiO_2, Heterogeneous catalyst, 2,4-thiazolidinedione, Condensation.

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Zinc oxide nano-powder catalyzed efficient synthesis of quinazolinone derivatives under solvent free conditions

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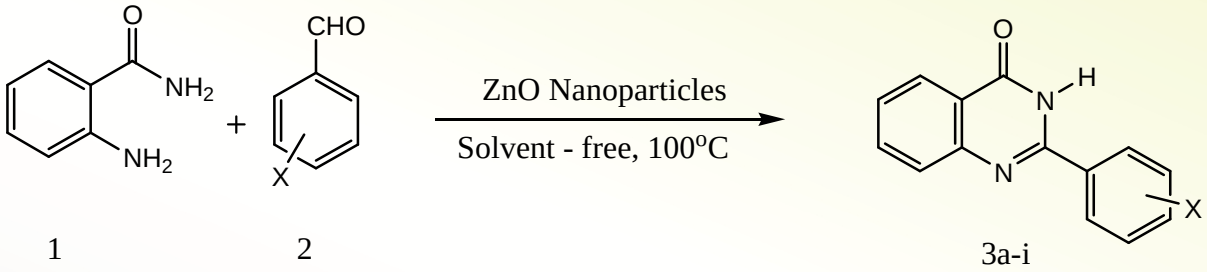
Abstract: Quinazolin-4(*3H*)ones is an important class of heterocyclic compounds widely occur in natural products, Ma et al [1]. They show a variety of biological and pharmacological activities including antibacterial, antifungal, antiviral, antimycobacterial,and antimalarial properties. Quinazolinone derivatives are also used as inhibitors of various enzymes, Zhang et al [2].

In view of the biological importance of quinazolinone and its derivatives, several synthetic strategies have been employed their synthesis. Classical routes for the synthesis of quinazolinone derivatives involving condensation of substrates such as anthranilic acids, halobenzamides, iminohalides, 2-halobenzonitriles or 2-nitrobenzonitriles, 2-aminobenzamides, amidines and isatoic anhydrides. Although reported methods are effective in many instances, they have one or the more disadvantages. Therefore, the development of general, efficient, simple and sustainable approaches is still desirable. In continuation of our work on ZnO catalyzed reactions, More et al [3], we report here a simple and efficient procedure for the synthesis of 2-substituted quinazolinone derivatives using zinc oxide nano-particals under solvent free condition.



1 2 3a-i

Scheme

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

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Environmental friendly efficient synthesis of benzimidazole and benzthiazole derivatives under aqueous medium

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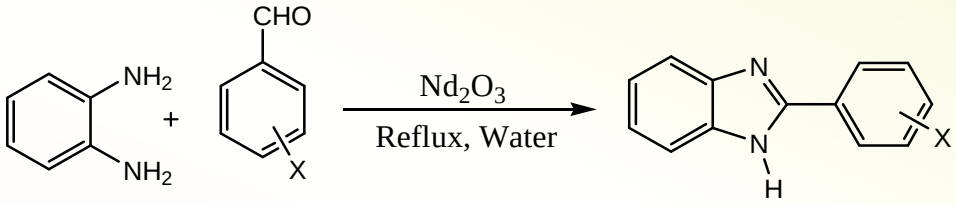
Abstract: Benzimidazoles and benzthiazoles are heterocyclic key structures in various biologically active compounds. They have shown different pharmacological activities such as antibacterial, antihypertensives, antiulcers, antifungals, antivirals, anticancers, and antihistaminics. Literature survey also indicataed that benzimidazole moiety can bind in the DNA minor groove, Ivanov et. al [1] and can act as a ligand to transition metals, Jayabharathi et.al [2]. Various methods have been reported for the synthesis of benzimidazole, benzthiazole or substituted benzthiazole derivatives by condensing *o*-phenylenediamines and *o*--aminobenzenethiol with acid chlorides or aromatic aldehydes. However, most of these methods have disadvantages, such as toxic reagents and catalyst, requirement of strong acidic conditions, long reaction times and tedious work up procedures.

In this communication, we wish to report a simple, environmentally benign and efficient method by condensation *o*-phenylenediamines or *o*--aminobenzenethiol with aromatic aldehydes for the synthesis of benzimidazole and benzthiazole derivatives catalyzed by neodymium oxide (Nd_2O_3) under aqueous medium.

Recycle and reuse of catalyst Nd_2O_3, use of water as a green solvent, short reaction time, simple work up procedure and excellent yield of products are the advantages this method.



1 2 Scheme 1 3a-j

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Uncatalyzed direct conversion of aldehydes into nitriles under aqueous medium

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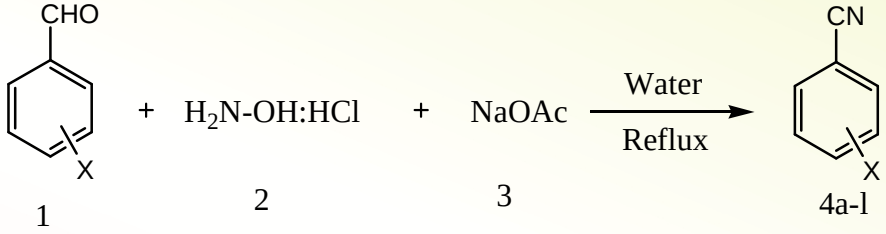
Abstract: Nitriles are versatile structural motifs in a number of pharmaceuticals, agrochemicals, , polymers, pigments, dyes and bioactive natural products, Brunton et. al[1]. Aromatic nitriles are used for preparation of amines, amides, amidines, carboxylic acid and nitrogen containing heterocyclic systems. The traditional approach for the synthesis of aryl nitriles usually involves dehydration of amides or oximes including Sandmeyer and Rosenmund-von Braun reactions, but these methods demand stoichiometric amount of cupreous cyanide reagents and pre functionlized starting materials. Recently, a verity catalysts like HMDS, CF3-BHA, TMSN3, ZrCl4/Pd/L, Zn(CN)2,TfOH, TFA, NH_4OAc, and sodium azide has been reported for the synthesis of nitriles. All these reported methods have one or other disadvantage, such as the use of expensive reagents, tedious workup procedures, toxic or hazardous reagent and solvents. More recently, Verma et. al [2] reported visible light-induced direct conversion of aldehydes into nitriles in aqueous medium using Co@g-C3N4 as photocatalyst. However, the method involves tedious procedure for preparation of catalyst and methanol based solvent system. Therefore, there is still scope to develop efficient and environmentally benign method. Herein, we describe a simple, efficient and uncatalyzed one-pot method for the synthesis of nitriles from aldehydes using water as a green solvent.



1 2 3 4a-l

Scheme 1

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P-55

Title: " Synthesis, characterization and biological activity of some new tert-butyl 4-5-Aryl-2-(furan-2-yl)-1H-benzo[d]imidazol-1-yl)piperidine-1-carboxylate derivatives"

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Abstract: A derivatives of new class of tert-butyl 4-5-Aryl-2-(furan-2-yl)-1H-benzo[d] imidazol-1-yl)piperidine-1-carboxylatehave been synthesized via 3 steps cyclization and coupling with different aryl boronic acids by using palladium catalyst.Moreover, synthesized of this targets done by coupling of tert-butyl 4-aminopiperidine-1-carboxylate with 1-fluoro-2-nitrobenzene by using TEA in ACN at 70oC for 16h. Reductive cyclization with sodium dithionate with MeOH:H2O(1:1) at 60^{o}C for 16h obtained in good to excellent yield. All this compounds was screened against antimicrobial activity.

Keywords: HATU, Reductive cyclization, suzuki coupling

P-56

DoE based Failure Mode and Critical Effect Analysis to Development of Eco-friendly and Economical Chromatographic Method for Estimation of Multiple Combined Formulations of Paracetamol

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ABSTRACT: DoE based failure modes and critical effect analysis was performed for development of HPTLC method for assay of multiple combined pharmaceutical dosage forms of paracetamol which offers optimised chromatographic condition to save time, solvent and cost of analysis. Failure modes were identified by prior knowledge of chromatographic method and listed in fish bone diagram. Failure mode were analysed for their critical effect on development of HPTLC method and criticality score given on bases of preliminary experimental trials. Identified potential failure modes were analysed for their effect on critical method attributes by DoE based screening design. Critically identified failure modes were linked with critical method attributes by DoE based response surface methodology. Effect of failure modes were mitigated by navigation of design space for development of HPTLC method having resolution more than 1.5 with tailing factor of each peak in chromatogram in range of 0.9-1.2. Finally chromatographic separation was performed on silica gel G F_{254} precoated on aluminium plate using Toluene: Ethyl acetate: Formic acid (6:4:0.1 v/v/v) as mobile phase with detection wavelength of 278nm. Developed method was validated for specificity, accuracy, precision, robustness, LOD and LOQ as per ICH guideline. Developed and validated method was applied for assay of multiple combined pharmaceutical dosage forms of paracetamol and results in agreement with published chromatographic method.

P-57

PLASMODIUM FALCIPARUM DIHYDROOROTATE DEHYDROGENASE (*PF*DHODH): A TARGET FOR ANTIMALARIAL DRUG DISCOVERY

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ABSTRACT: Malaria is themost severe disease all around the world and several kinds of research for the identification and optimization of hit to lead as antimalarial agents. Alarge number of drugs are available for its treatment, however, the development of resistance has become more widespread with most of the antimalarial drugs.One of the most severe species is *Plasmodium falciparum* and nowadays at a pre-erythrocytic stage for inhibiting the multiplication of poisoned liver cells which contain *plasmodium* parasites here one of the strongest and important targets for inhibiting malaria disease is *Pf*DHODH. Dihydroorotate dehydrogenase inhibitorsare one of the strongest lead molecules for inhibiting malaria parasites.There are several reviews and research work done by a scientist, reviews based on main responsible ring structure their substitution several different type ring and hit to lead molecules identified which are showing inhibitory concentration very potent and that proved as a successful hit to lead molecule for drug discovery of antimalarial drugs. *Pf*DHODH inhibitorsare new hope for reducing and inhibiting cell growth of malarial parasites and lead moleculeshave specific binding site to the amino acid that proved as specific binding to enzyme and responsible for antimalarial activities based on different ring structure. This review will be helpful for researcher, students for furtherdevelopment of *Pf*DHODH inhibitors as antimalarial drugs.

P-58

TO STUDY THE REGULATORY REQUIREMENTS FOR EXPORT OF PHARMACEUTICALS BY MERCHANT EXPORTER WITH EMPHASIS ON CONTRACT MANUFACTURING REQUIREMENTS IN INDIA, USA AND EUROPE

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ABSTRACT: The Indian Pharmaceutical market is the third largest and eleventh largest in terms of volume and value, respectively. India is the largest provider of generic drugs globallyaccounting for 20 percent of global exports. India has gained a foothold in the global arena with reverse-engineered generic drugs and APIs. India has the highest number of manufacturing facilities approved by USFDA. The market is expected to grow to USD 55 billion by 2020, thereby emerging as the sixth largest pharmaceutical market globally. It is said "Every third pill consumed in the world is made by an Indian manufacturer" which explains the potential of the contract manufacturing parties in the Healthcare System of the world. The generics market size in USA has increased from USD 47 billion in 2012 to USD 71 billion in 2017 which will still rise. This market size of the generics in USA is majorly dependent on the patent of the drug. Within the past five years, drugs worth USD 83 billion have gone off-patent with another USD 72 billion will be slated off in the coming five years. Europe shared 228.1 billion euros globally in the pharmaceutical market till 2011. The size of the Europe market is estimated to grow by 25% between 2017-2022 with the CAGR of 4.5% over this period. Thus each country has equal share in manufacturing and export of pharmaceuticals for both generics and innovator. Here, we tried to compare regulatory requirements for export of pharmaceuticals in India, US and Europe.

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P-59

Method development on Ibrutinib and its Impurities Characterization by HPLC

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Abstract: A single robust, simple, precised, and accurate HPLC method was developed for the validation and impurity characterization. Ibrutinib is a small molecule drug that bind to a protein used to treat B cell cancer like lymphoma for that the impurity is characterize by an HPLC method. A discriminatory, novel and an accurate precised reverse phase high performance liquid chromatographic method (RP-HPLC) with UV was established and validated for the detection of impurities G and M. Chromatographic conditions used were Poroshell 120EC C-18,(150*4.6)mm, 2.7µm Agilent. Mobile phase A prepared were mix buffer solution and acetonitrile in the ratio of (900:100) and the Mobile phase B in the ratio of (700:300). Column temperature is 55 ˚C with UV detection at 210 nm volume injected is at 10 µl runs at 60 min. System suitability solution would be according to the accurately weigh of ibrutinib system suitability mixture according to an acceptance criteria. Inject 10µl of the six replicate if the standard solution into the chromatograph to set the chromatographic conditions and set the record chromatogram of the HPLC. The method was also evaluated for the accuracy, linearity, limit of quantification and stability. Advanced HPLC technology have improved competency for ibrutinib drug impurity profiling in relations of faster analysis, better seaprations in the recorded chromatogram and precised quicker method development. Therefore, it is essential to characterize the impurities G and M in ibrutinib by the HPLC method.

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P-60

A novel approach towards the synthesis of pyridazine derivatives

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ABSTRACT: Pyridazines are six membered heterocyclic aromatic structures having two nitrogen atoms. These compounds are comparatively less explored than its other isomeric diazines specially pyrimidines because pyridazines are not easily produced by biochemical nitrogen transformation in nature and therefore its availability in nature is not known. Most of the preparation methods of pyridazine derivatives involves condensation of activated carbonyl compounds with hydrazine hydrate or its derivatives [1].These condensations are also carried out by using ionic liquids. Pyridazines are known for its variousmedicinal properties such as analgesic, antibacterial, antidepressant, anti-diabeticetc.It is also explored by the agrochemical science for the synthesis of insecticides, fungicides, cardiotonics, and bacteriocides [2] In the present work, simple method and starting material has been used for the synthesis of pyridazine. 2, 4 Dintrophenylhydrazones are subjected for the cyclisation in presence of simple alkali bases for the preparation of pyridazine derivatives. The method avoids use of toxic and hazardous hydrazine hydrate for the preparation of pyridazine derivatives.

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P-61

Prediction, preparation, characterization, and evaluation of brexpiprazolecocrystal: a compelling case of stability improvement by cocrystallization

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ABSTRACT: Brexpiprazole (BREX) is a well-known drug used in the treatment of the atypical psychotic disorder. BREX undergoes oxidative degradation in the presence of excipients like polyvinyl pyrrolidone (PVP) and forms N-oxide impurity. Hence the present study aimed towards the development of cocrystals of BREX to address stability concerns along with the improvement of solubility and dissolution. Nearly 13 coformers were evaluated for cocrystal formation with BREX using the prediction model, followed by experimental verification of results using the solution cocrystallization method. Prediction study showed that hydroxyl or carboxyl group-containing coformers formed a hydrogen bond with the piperazine ring of BREX. Differential scanning calorimetry (DSC), powder X-ray diffraction (PXRD), hot stage microscopy (HSM), and Raman spectroscopy analysis confirmed the formation of a cocrystal of BREX with succinic acid and catechol. Further, single-crystal X-ray diffraction (SCXRD) of Brexpiprazole-catechol (BRC) cocrystal confirms that it crystallizes in monoclinic space group *P21/C*. BREX is known to exhibit photo-instability on granulation with the most commonly used binder, polyvinylpyrrolidone (PVP), in wet granulation. BRC cocrystal and plain BREX granulated with PVP as a binder and the chemical stability of the granules were investigated. Plain BREX showed oxidative degradation and formation of *N*-oxide degradation products under stability conditions within 7 days. However, the BRC cocrystal displayed superior stability against stability conditions because the reactive site in the piperazine ring of the BREX moiety was blocked due to the hydrogen bond between the drug and co-former.

P-62

Development and validation of HPTLC method for simultaneous estimation of Mirabegron and Solifenacin succinate in its synthetic mixture

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ABSTRACT: The present study was designed to develop a precise and accurate HPTLC method for simultaneous estimation of Mirabegron and Solifenacin succinate in its synthetic mixture. The chromatographic separation was performed using aluminum backed pre-coated with silica gel 60F254 as stationary phase and n-Butanol: Acetone: Water: Ammonia (6: 4: 0.1: 0.2 % v/v/v/v) as mobile phase. The quantification was carried out at wavelength of 221 nm. The method was validated as per ICH Q2 (R1) guideline. Rf value of Solifenacin succinate and Mirabegron was found to be 0.23 ± 0.02 and 0.78 ± 0.02 respectively. Linearity was found in the range of 1000-5000 ng/band and 2500-12500 ng/band for Solifenacin succinate and Mirabegron respectively. Correlation coefficient for both Solifenacin succinate and Mirabegron was found to be 0.996. The LOD and LOQ for Solifenacin succinate was found to be 181.40 ng/band and 549.70 ng/band respectively and for Mirabegron the LOD and LOQ was found to be 176.80 ng/band and 535.76 ng/band respectively. Percentage recovery was found to be in range of 99.65–100.32% for Solifenacin succinate and 100.10–101.25% for Mirabegron.

P-63

The clinical manifestation of polycystic ovarian syndrome and its association with various risk factors.

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Abstract: To determine age wise prevalence, clinical characteristics of PCOS in women of reproductive age in Ahmedabad region and determination of associated risk factors in development of PCOS was carried out.A cross-sectional study was conducted among 150 women, the age of 20-45 years who visited the two hospitals enrolled in the study. PCOS was diagnosed if both menstrual dysfunction and clinical hyperandrogenesim was detected as per Rotterdam criteria, with determined association of PCOS with obesity and overweight, socioeconomic status, physical activity and other risk factors using pre-tested and pre-designed questionnaire. A 123 out of 150 women were diagnosed as PCOS according to the Rotterdam criteria. The highest prevalence of PCOS was found at age group of 30-34 yr. The significant correlation was found between hursutisum, acne with PCOS but not with blood pressure and prolactin level. In our study, the prevalence of obesity in PCOS women was found to be higher. We also found that higher percentage of PCOS women were having a family history of diabetes mellitus and presence of dysmenorrhea. The higher percentage of PCOS women belong to upper socioeconomic class with having less physical activities.We concluded that the higher prevalence of PCOS observed at the age between 30-34 years. The menstrual irregularity, hursutisum, dysmenorrhea and acne were clinical characteristics of PCOS. Obesity, physical inactivity and the family medical history of diabetes mellitus were observed to be significantly associated risk factors with PCOS.

P-64

SOLID AS SOLVENT"- NOVEL TECHNIQUE FOR SPECTROPHOTOMETRIC ESTIMATION OF METRONIDAZOLE TABLETS USING SOLIDS (EUTECTIC LIQUID OF PHENOL AND METFORMIN HYDROCHLORIDE) AS SOLUBLIZING AGENT (MIXED SOLVENCY CONCEPT)

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ABSTRACT: The eco-friendly method in the field of drug has been given by Maheshwari for the estimation and formulation precluding the use of toxic organic solvent. The present research work also provides a novel method to estimate spectrophotometrically, the Metronidazole drug, in tablet formulations without the use of organic solvent. In this investigation, an attempt was made to show that solids can also be wisely used for forbidding organic solvents. The main objective of the present study is to demonstrate the solvency of solid. In the present study, a eutectic liquid (PMHCl 41) obtained by triturating phenol crystals and Metformin hydrochloride in 4:1 ratio on weight basis was employed to extract (dissolve) metronidazole from fine powder of tablets. Distilled water was used for dilution purpose to carry out spectrophotometry estimation at 320nm without utilizing any organic solvent. The solubility of metronidazole in distilled water at room temperature was found to be 7.28 mg/ml. while the solubility of metronidazole in PMHCl 41 was more than 130 mg/ml i.e., 18 times approximately. Proposed spectrophotometry analytical method is novel, rapid, free from toxicity of organic solvent, accurate and reproducible. The recovery studies and statistical data confirmed the accuracy. Phenol, Metformin hydrochloride and the tablet excipients did not interfere in the spectrophotometric estimation at 320nm.

Keywords: Mixed-solvency concept, metronidazole, phenol, metformin hydrochloride, spectrophotometric analysis, eutectic liquid.

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Emerging role of nanoparticle using herbal extract in Alzheimer's disease

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ABSTRACT: The treatment of CNS disease always remains challenging. Alzheimer's disease (AD) is a neurodegenerative disorder that causes dementia in the brain often leads to loss of neurons. The clinical signs are impaired memory, behaviour, language, difficulty in judgement and decision making. The pathophysiology of AD includes deposition of β amyloid plaques, accumulation of neurofibrillary tangles and oxidative neuronal damage. More than 4 million people in India are suffering from some form of dementia. Nature is a rich source of phytoconstituents derived from herbal plants. The use of herbal medicine prevents forgetfulness and improves memory. In the era of modern Ayurveda, herbal medicines become the most upcoming blockbusters to target CNS. The use of herbal medicine improvises the treatment by giving maximum benefits and minimum side effects. The herbal extract of the plant is used as the major source for the formation of herbal drug. The conventional therapies often have major drawbacks of poor solubility, lower bioavailability, and ineffective ability to cross blood brain barrier (BBB). Nanoparticles overcome the drawbacks of conventional therapy. Different hallmarks of nanoparticles are lipid-based NP, metal-based NP, polymer-based NP, nanoemulsion, microemlusion, liquid crystals, etc. The nanoformulation made using herbal extract improvises the treatment than the current conventional therapy. Thus, nanoparticle plays a very crucial and important role in the treatment of Alzheimer's disease.

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P-66

REGULATORY COMPLIANCE MANAGEMENT OF TRANSDERMAL PATCHES

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ABSTRACT: Regulatory affairs (RA) professionals play critical roles in a pharmaceutical industry because it is concern about the healthcare product lifecycle, it provide strategic, tactical and operational direction and support for working within regulations to speed up the development and conveyance of safe and effective healthcare products to individuals around the world. Regulatory compliance is adherence with different laws, regulations, guidelines and specification relevant to process. Violation of such regulations may prompt lawful disciplines. Regulatory compliance describes the goal that organizations aspire to accomplish in their efforts to ensure that they are aware of and take steps to fulfil with relevant laws, policies, and regulations. The pharmaceutical industry is highly regulated industries in our country and is dealing with human life, so adherence with the regulation and regulatory guidelines must require. Transdermal Patches are now becoming widely used drug delivery system. The current scenario shows that the ration of generic drug is double than new drug. Transdermal Patches are at the third place after oral and Injectable in the category of widely used pharmaceutical products worldwide. There are only 54 Transdermal patches available in the market from which
28 are new patch and 26 are generics. Drug delivery systems plays crucial role in Pharmaceutical Research and Development. To promote the efficiency of drug and extend the life cycle of product, quantitative analysis of approval process and knowledge of the technical barriers must require.

KEYWORDS: Transdermal Patch, Guidelines & Regulation, Lifecycle Management, Regulatory compliance

P-67

Synthesis and CrystalStructure Studies ofPyranone-Isoxazole Fused Scaffold

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ABSTRACT: crystal packing,anti-HIV,supramolecular,non-covalent interactions, isoxazole Pyranone-Isoxazole fused molecules weresynthesized by the result of scaffold transformation from 4-(hydroxyamino)-2-oxo-6-aryl-N-(substituted)-2*H*-pyran-3-carboxamide. Hydroxylamine efficiently substitutes the thiomethyl group at 4-position on pyranone-3-carboxamide.Further, the basic condition induces intramolecular ring transformation and yielded a fused ring compound.The presence of isoxazole moiety is a major core in our molecular design process. Moreover, this class of molecules has shown excellent biological activities like anti-inflammatory, anti-convulsant, anti-cancer and anti-HIV activity, and opens a scope to explore further in therapeutic applications. X-ray quality single crystal of the compound was prepared by a slow evaporation method using methanol as solvent. Non-covalent interaction was studied to understand the conformation of the final compounds. The crystal packing studies reveal the intermolecular packing pattern in 3D-space, which provides an opportunity to understand the supramolecular system.The weak non-covalent forces including hydrogen bonds and pi-interactions were studied in the crystal packing system.

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Expedited Regulatory Review in the US, the EU, and Japan

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Abstract: There are standard regulatory procedures to review the application submitted to an agency. Every particular regulatory authority has specific review procedure for reviewing the application. Here, US has USFDA (Food and Drug Administration), EU has European Medicines Agency (EMA) and Japan has Pharmaceuticals and Medical Devices Agency (PMDA). But some dosage forms are very critical and their approval need according to the affected population of the country leads to frame other review process for fast availability of drug treatment. Again every particular country has different process for other product's need. The Food and Drug Administration (FDA) first developed the breakthrough therapy designation, and then the Pharmaceuticals and Medical Devices Agency (PMDA) and European Medicines Agency (EMA) introduced the Sakigake designation and the priority medicines (PRIME) designation respectively. Each process is not completely different from each other but poster will focus on things which are important from particular regulatory authority perspective. The poster will define the review processes, requirements to undergo such review process and features of that process.

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Quantification OfBimatoprost In Pharmaceutical Formulation Using High-Performance Liquid Chromatography

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ABSTRACT: Simple, precise and economical RP-HPLC method has been developed for the estimation of Bimatoprost in ophthalmic solution. Chromatography was carried out on Hypersil BDS C_{18} (250 x 4.6)mm, 5µ, using a mixture of formic acid buffer (pH 2.6 ± 0.05) and acetonitrile (80:20 v/v) at a flow rate of 1 ml/min with injection volume of 100µL. Detection was performed at 210nm at 40˚C. The retention time was found 5.68 minutes. The run time was 10 minutes. The linearity range was between 0.5 – 20 µg/ml. The proposed method provides accurate and precise quality control tool for routine analysis of Bimatoprost in ophthalmic solution.

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Electrochemistry and Neurotransmitter

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ABSTRACT: Neurotransmitters are chemicals which behave as messengers in the synaptic transmission process. Neurotransmitters are important for human health. Sometimes activities of neurotransmitters become imbalance and causes serious mental diseases like Parkinson's disease, schizophrenia, and Alzheimer's disease. That's why we have to monitor the concentration of neurotransmitters. Chemical signaling during liberation of neurotransmitters into the extracellular space is the most important means of communication between neurons. In this review, we give a general idea of the fundamental principle of constant-potential amperometry and fast-scan cyclic voltammetry, usually employed electrochemical methods, and the general purpose of these methods to the study of neurotransmission and with the help of above methods we can monitor the concentration of neurotransmitters like dopamine, norepinephrine, and serotonin and their metabolites. This review gives particular electrochemical method for particular neurotransmitter and sometimes sensor is also helpful to detect concentration of neurotransmitter along with method like biochemical sensor to detect dopamine.

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3D QSAR Studies ofImidazo[1,2-*a*]pyrimidin-5(1*H*)-one and 1,2,4-Triazolo[1,5-*a*]pyrimidin-7(3*H*)-one Derivatives as Phosphoinositide 3-Kinase (PI3K)-β Inhibitors

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ABSTRACT: The phosphoinositide 3-kinase (PI3K) has emerged as an attractive target for targeted cancer treatment because of its aberrant activation in various cancers. In the present study, CoMFA and CoMSIA study were performed on the series of imidazo[1,2-*a*]pyrimidin-5(1*H*)-one and 1,2,4-triazolo[1,5-*a*]pyrimidin-7(3*H*)-one derivatives for the identification of essential structural features of selective PI3K-β inhibitors responsible for anti-cancer activity. The analyses were performed using SYBYL X software and best CoMFA and CoMSIA models were obtained by means of Distill rigid body alignment of training and test set compounds. TheCoMFA and CoMSIA models were found statistically significant with cross-validated coefficients (q^2) of 0.598 and 0.570, respectively and reliable in terms of prediction results.The derived contour maps from 3D-QSAR models revealed that steric and hydrophobic fields played important roles in determining the inhibitory activity of PI3K-β inhibitors. The output of the present study may provide better insight into designing of new potent compounds of PI3K-β inhibitors as anticancer agents.

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USE OF ACTIVATED CHARCOAL IN WASTEWATER TREATMENT

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ABSTRACT: Nowadays water pollution is major problemin public health. Wastewater includes any unwanted material that could pollute our fresh water system including sewage, sludge, waste water from domestic use, dairy, chemical industries etc. The water becomes turbid and contaminated with chemical and biological factors. The activated charcoal is used in the removal of most difficult impurities from wastewater. In the present study the charcoal powder is used for reduction of turbidity of wastewater. TDS, DO, sodium is reduced by charcoal treatment. 20 mg of charcoal per litre decolorized the waste water in 24 to 30 hours. Our results showed that,activated charcoal powder has a better efficiency to reduce the pollutant loads in liquid discharges. Odour of wastewater diminishes by charcoal treatment. After charcoal treatment DO of wastewater is increased and BOD, COD is reduced to considerable level. Acidic nature of waste water is changed to neutral to slightly alkaline after charcoal treatment. In conclusion, charcoal treatment is effective for remediation of wastewater for agricultural and other purposes.

Keywords: Wastewater, Charcoal powder, DO, Turbidity, Acidity

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COMPARATIVE EVALUATION OF TIZANIDINE AND BACLOFEN IN SPASTICITY

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ABSTRACT: The objective of the study was to evaluate and compare the efficacy of tizanidine and baclofen in combination with physiotherapy for the treatment of spasticity associated with stroke, SCI. Three hundred and sixty six patients with spasticity due to post stroke and SCI were enrolled in the present study that was conducted both retrospectively and prospectively. We evaluated the efficacy of each muscle relaxant and physiotherapy from baseline to 8 weeks using different scales. In terms of improvement of the muscle tone both tizanidine and baclofen caused a significant improvement in the muscle tone but their effect was short lived as compared to physiotherapy. In terms of reducing the spasm frequency, baclofen was effective as physiotherapy and only showed improvement at week 8. When tizanidine was compared to baclofen, tizanidine caused a significant reduction in the frequency of muscle spasm was seen at week 4 and week 8.In terms of improving the pain, baclofen caused a short term improvement whereas tizanidine showed a greater efficacy in terms of reduction of pain as compared to both physiotherapy and baclofen.In terms of improving the muscle strength, both tizanidine and baclofen were as effective as physiotherapy. In terms of improving the functional outcomes, both tizanidine and baclofen were found to be equally effective as compared to the physiotherapy. In conclusion, our data suggests that baclofen and tizanidine offer no greater advantage than physiotherapy in terms of improvement of muscle tone, muscle strength and spasm frequency.

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FANCONI ANEMIA: A MULTISYSTEM DISORDER

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ABSTRACT: Fanconi anemia (FA) is a rare autosomal recessive cancer susceptibility genetic disorder, characterized by various congenital abnormalities, progressive bone marrow failure, and predisposition to malignancies and affects multiple organs of the body. FA patients are hypersensitive to inter-strand DNA cross linking agents such as diepoxybutane, mitomycin C and other ionizing radiation and thus, FA is diagnosed by chromosomal breakage test. The eight FA genes (for subtypes A, B, C, E, F, G, L, and M) form a core protein complex which contains FANCA, FANCC, FANCF, and FANCG proteins and is required for the activation of the $FANCD_2$ protein to a mono-ubiquitinated isoform. In normal cells, $FANCD_2$ is monoubiquitinated in response to DNA damage and is targeted to the site of DNA double strand break. Activated $FANCD_2$ protein further recruits cluster of a protein and one of this protein is the breast cancer susceptibility protein, BRCA1, in ionizing radiation–induced foci and in synaptonemal complexes of meiotic chromosomes. The DNA double-strand break requires BRCA1 and BRCA2 for homology-directed DNA repair (HDR) in G_2 and S phase.The loss of BRCA functions leads to uncontrolled growth and spread of abnormal cell and causes cancer. Mutation in any of these genes interferes FA mediated DNA repair pathway. Biallelic mutation in BRCA1 causes a new Fanconi anemia subtype. Bone marrow transplantation is the only known cure for the hematologic manifestations of FA. Various other methods of treatment and management of Fanconi anemia may include Gene therapy, androgen therapy, etc.

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Prospects of Nano-Formulations for Managing Dry Eye Disease (DED)

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ABSTRACT: Ocular disorders encompass a multitude of diseases that are unique in their cause, therapy and degree of severity. Due to distinctive morphology of the eye, efficient ocular drug delivery has proven to be a difficult task[1]. Components of the ocular surface synergistically contribute to maintaining and protecting a smooth refractive layer to facilitate the optimal transmission of light. Dry eye can damage the ocular surface and result in mild corneal epithelial defect, to blinding corneal pannus formation and squamous metaplasia[2]. Significant progress in the treatment of dry eye has been made in the last two decades; progressing from lubricating and hydrating the ocular surface with artificial tear to stimulating tear secretion; anti-inflammation and immune regulation. Novel drug delivery systems have several advantages over conventional multi dose therapy. For the past few decades, there has been a considerable research interest in the area of nano-particulate drug delivery systems[1]. The aim of this poster is to provide a brief overview of the emerging treatment options for dry eye syndrome involving nanoparticulate formulations, and discussions towards the future prospects of nano-formulations in the mainstream of ophthalmic diseases.

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MIND THE GAP: INVESTIGATING THE ROLE OF COLLECTIVE ACTION IN THE EVOLUTION OF INDIAN MEDICAL DEVICE REGULATION

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ABSTRACT: Research is of case study of Indian medical device sector, it examines the growth and development of regulations of medical devices and its regulatory frameworks, thereby analyzing circumstances, factors and processes of development through which regulatory domain for technological industry factors are explained. It tries to off-load the complex correlation of industrial competence and possibilities of technology in healthcare sector and nurturing human health. It attempts to provide facilities and and also regulate inclusive development of technology in healthcare field in emerging countries. The research paper explains the lack of action in regulation that can critically affect and also slows down the growth of technological regulation of medical devices thereby affecting growth of medical device industries particularly in developing countries. It suggests that affiliation of different stakeholders is the to success of institutional change in regulation of medical devices. These research findings provides significant suggestions to the developing countries which are lacking behind in regulation and evolution in healthcare sectors specifically in technology related development in healthcare field and provides implications in related context and needs.

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Development of EEG Biomarker for Alzheimer's Disease

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ABSTRACT: Alzheimer's disease is a neurodegenerative disorder that progresses with age. It is characterised by intellectual and cognitive disturbances which worsens with age. The neuropathology of Alzheimer's includes neurofibrillary tangles and formation of plaques. Early detection may help to control the symptoms and to decide the right treatment which may slow down the process. Various biomarkers can be used as diagnostic agent for the early detection. Electroencephalogram is widely used as biomarker for Alzheimer's disease. EEG is an electrophysiological monitoring method to record the electrical activity of brain. EEG can be used to distinguish between patients with Alzheimer's or mild cognitive impairment. The hallmark of EEG abnormalities in AD patients is a shift of the power spectrum to lower frequencies and a decrease in coherence of fast rhythms. [1] Although EEG fails to meet the criteria of ideal biomarker in the terms of complexity in use, design and implementation, but it still is reliable, non invasive, effective and cost efficient imaging tool for early detection of Alzheimer's disease. [2]

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New World of Biosimilars:An Emerging Market Opportunity in India

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ABSTRACT: In Recent years, there are many blockbuster Biological products going off patent which has generated an abbreviated route for the Biosimilars products also known as “follow on biologics” or “similar biologics” which relies on the extensive comparability testing against Reference Biological Products (RBP) swearing product’s quality, safety and efficacy. Thus, they require discrete marketing approval with plentiful documentation as they are not generic version of biologics.The first draft guideline for Biosimilars was established by Europe, subsequently Japan and USA have developed the draft guidelines. While recently, India’s first guidelines were imposed in 2012, with amendments in 2016. India has vigorous Pharmaceutical Industry for the generic drug while it can become an emerging market for the Biopharmaceutical drug.Biological medicines are biotechnology developed drugs having large molecule which is complex in nature and are very sensitive to manufacturing conditions and parameters. Even a slight change in manufacturing conditions changes the quality and safety aspects of end product owing to increased risk for immuneresponse. Thus, there is need for stringent regulatory guidelines. Biosimilar drugs have moderate marketing cost which is fascinating and generally 40 to 50 % less to that of originator drug product. The biosimilar market will soon be thriving above $80 billion price of drugs in next seven year.

Keywords: Biologics, Cost-effective,Manufacturing, Safety, Market.

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Physiologically based pharmacokinetic (PBPK) modeling to predict pharmacokinetic profile of Abiraterone Acetate

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ABSTRACT: Modeling is an essential tool in pharmaceutical formulation development. It can save both time and money, as well as facilitate decision process at critical points in formulation development. Predicting pharmacokinetic profile of a drug substance, using *in-vitro* drug release and solubility, in actual physiological environment is very challenging due to vast number of *in-vitroin-vivo* variables involved.

Various methods like convolution are used for predicting pharacokinetic profile of drugs from *in-vitro*drug release profile. These methods only take into account the physicochemical characteristics of the drug (particle size, solubility, etc.), but fail to consider the physiological conditions (gastrointestinal motility, fluid volume, etc.).

Physiologically based pharmacokinetic (PBPK) modeling is a compartment and flow-based type of pharmacokinetic modeling using mathematical modeling technique to predict absorption, distribution, metabolism and excretion (ADME) of drug substances in humans and other animal species.PBPK models are compartmental models and have advantage over classical pharmacokinetic models which are less grounded in physiology. PBPK modeling using STELLA® software considers both physicochemical characteristics of drug substance and physiological conditions in conjunction with pharmacokinetics of the drug to predict the plasma profile.

Pharmacokinetic profile of Abiraterone Acetae, molecule with solubility and permeability limitations, has been predicted using a two-compartment model with first-order elimination. In addition, a sequential zero- and first-orderabsorption process using transit compartment was applied to describeand account for the delay in thesystemic absorption of the drug. *In-vitro* drug release and solubility results were coupled with *in-silico* PBPK modeling to predict plasma profiles.

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Design, Synthesis and Pharmacological Evaluation of Small Molecules targeting Histone Deacetylase Inhibitors (HDAC) as Anti-Cancer Agents

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Abstract: Despite many advances in prevention and treatment of cancer, the ability to cure cancer is still in urgent need to develop effective drug therapy. Current cancer chemo therapeutics is primarily less effective due to the lack of selectivity and specificity for targeting cancer cells over other cell. Therefore, design and synthesis of new effective, selective and less toxic anticancer therapy one of the most pressing health problems.

Histone deacetylase inhibitors (HDIs) are emerging as a new class of anticancer agents and have been shown to alter gene transcription. In the present study, a series of novel histone deacetylase (HDAC) inhibitors using the tetrahydro-1-benzothiophene (1) as the capping group were designed and synthesized.

Keyword: Histone, HDAC, Benzothiophene

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MICROWAVE ASSISTED ACCELERATED STABILITY STUDY OF AMLODIPINEBESYLATE

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Abstract: Stability studies are important to ensure drug product quality and stability until the time of consumption by patients.Real-time stability studies are time-consuming therefore accelerated stability studies are performed at elevated temperatureto catalysed the rate of reaction.According to the International Conference on Harmonisation (ICH) guidelines, accelerated stability studies are performed at 40ºC ± 75 % relative humidity (RH) for 6 months. The process of microwave heating is used in synthetic chemistry for last few years to increase rate of reaction and does reducing the time of synthesis. The use of microwave to carry out accelerated stability studies rather than the conventional method may reduce the time for predicting the stability of the drug product.The aim of the present work was to evaluate the feasibility of the microwave assisted heating technique in the prediction of drug stability.In the present work, an attempt was made to carry out accelerated stability study of amlodipine besylate (AMD) using microwave heating and conventional method. The degradation profiles from both the methods were compared to correlate the results. The AMD samples were placed in the stability chamber at 40ºC ± 75 % RH and were collected at pre-defined time intervals i.e. 0,1,2,3,4,5 and 6 months. Similarly, samples were also kept in microwave synthesizer at different conditions i.e. power ranging from 200 W to 600 W; temperature ranging from 100 ˚C to 160 ˚C. The drug degradation patterned was determined using high-performance liquid chromatography. The chromatographic profiles obtained from microwave-assisted technique was then compared to the conventional method. The study demonstrated a substantial correlation between conventional and microwaveassisted stability. The microwave-assisted stability study under conditions with (50µL water; 400W; 160T; 15min) showed total 6 common degradation product in mixture with glucose to that of the conventional method. Similarly, microwave-assisted stability study under conditions with (50µL water; 200W; 160T; 15min) showed 3 common degradation product in mixture with lactose and (80µL water; 400W; 100T; 15min) showed 3 common degradation product in the tablet as compared to the conventional method. Therefore, to conclude, microwave-assisted heating is an efficient way to perform the accelerated stability study of APIs and formulations.

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Current studies of analytical method for the determination of Gefitinib

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Abstract: Cancer is the unrestrained growth of abnormal cells anyplace in a body. These abnormal cells are termed cancer cell, malignant cells,or tumor cells.Lung cancer is the **uncontrolled growth of abnormal cells** in one or both lungs. Lung cancer is classified into two types: (1) small cell lung cancer and (2) non-small cell lung cancer. In 2018, over two million new lung cancer cases and 1.7 million deaths were estimated to occur worldwide, representing 14% of the new cancer cases and 20% of the cancer deaths. Gefitinib (Iressa) is the first quinazoline-based epidermal growth factor receptor's (EGFR) tyrosine kinase inhibitor (TKI) to be approved for the treatment of cancer. Gefitinib is a oral treatment for non small cell lung cancer (NSCLC) that has spread into the surrounding tissues (locally advanced) or to other parts of the body. Tyrosine kinase is a protein that sends signals directing cancer cells to grow and gefitinib block these signals. There were many analytical method was used for the determination of gefitinib like a simple and rapid reverse-phase high-performance liquid chromatographic (RP-HPLC) method was developed and validated for the simultaneous separation and estimation of gefitinib (an anti-cancer drug) and its process-related impurities. Rapid resolution liquid chromatography (RRLC) method was used for the stress studies and quantitative determination of related substance and assay. IR spectroscopy, UV spectroscopy, and bioanalytical method development like HPLC and LC-MS method was used.

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VACCINE SAFETY VIGILANCE

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Abstract: A vaccine is a biological preparation that provides active acquired immunity to a particular disease.A vaccine typically contains an agent that resembles a disease-causing microorganism and is often made from weakened or killed forms of the microbe, its toxins, or one of its surface proteins.Reporting of adverse events following immunization (AEFI) is a key component for functional vaccine safety monitoring system.AEFI reporting is important to post-marketing vaccine safety surveillance and has the potential to identify new or rare AEFIs, shows increase in known AEFIs, and help to maintain public confidence in vaccine programs.Knowledge of background rates are especially useful when a new vaccine is introduced or a schedule change is made. Signal and events associated with newly introduced vaccine and AEFI that may have been caused by an immunization error should be reported during vaccine pharmacovigilance. There are criteria for establishing causality aftervaccine-related adverse events. There are well established criteria for causality assessment of adverse events related to pharmaceutical products, ofwhich dose responsiveness and rechallenge are among the major planks, theycannot be applied to vaccines. However, other criteria, such as biological plausibility and laboratory evidence of vaccineinvolvement, can assume greater importance for vaccines than for non-biological agents. Vaccines safety vigilance is an important matter in regulatory approval as all vaccines are not safe enough and hence special emphasis should be laid on regulatory framework so that benefits outweighs risks.

Keywords: Causality, Signal, AEFI, Rechallenge, Plausibility, Pharmacovigilance

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FORMULATION DEVELOPMENT OF ANTI-EMETIC LOZENGES FOR TREATMENT OF MOTION SICKNESS

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Abstract: The plethora described in this abstract directs towards the development of an antiemeticlozenges of meclizine hydrochloride for the treatment of motion sickness. Motion sickness is one of the most common disorder and many people suffer from motion sickness and are reluctant to take wide tablets or doses for treatment of it. Meclizine is choice of drugs for treating motion sickness but is available in tablet dosage form today. This possess following problem of slow onset of action and hence effect takes time. Development of a lozenge-baseddosage form will lead to increase in the availability of drug and thus increases the dissolution and onset of action of drug as the drug is readily available in circulation. Also, lozenge dosage form provides great patient acceptability and compliance due to wide flavours and shape. Thus, this research focusses on solubility enhancement of BCS class 2 drug and formulation of lozenge-based dosage form that will help the patients worldwide with motion sickness.

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ANALYTICAL APPROACH FOR COMBINATION OF SIMVASTATIN AND FENOFIBRATE IN MIXED HYPERLIPIDEMIA

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ABSTRACT: In today's world, hyperlipidemia has become an emerging disease, due to modern life style of people. In mixed hyperlipidemia the level of both Low Density Lipoprotein (LDL) and High Density Lipoprotein (HDL) increases, which give rise to a very risky disease known as Coronary Heart Disease. Till now many drugs from the statins class has been developed worldwide. There are also many analytical techniques such as HPLC (High Performance Liquid Chromatography),HPTLC (High Performance Thin Layer Chromatography), LC-MS (Liquid Chromatography coupled with Mass Spectroscopy), and UV, NMR, FTIR were developed respectively. Simvastatin and Fenofibrate drugs from the class statins and fibrates are used in combination for the treatment of mixed hyperlipidemia. Combination of these drugs are selected because statins only lower the LDL levels in blood but it does not have any effect on HDL levels. So it is used in combination with Fenofibrate to lower the HDL and LDL levels in blood stream. Only this combination of fibrate class do not alter the metabolic pathway of statin and hence, it is safe to use.

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ROCK: A POTENTIAL ENZYME IN CANCER

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ABSTRACT: Cancer is associated with cellular changes, such as increased migratory potential, modified cell-cell contact and generation of cellular forces, these are associated with alteration of cytoskeleton. Rho-associated protein kinase (ROCK) is a kinase belonging to the AGC (PKA, PKG, PKC) family of serine-threonine kinase. Main two kinases, ROCK I and II, are key regulators of actin cytoskeleton. ROCK is associated in progression of cancer and in certain cancer rock protein expression is elevated. ROCKs exist in closed conformation and are activated by binding with guanosine triphosphate (GTP). Number of ROCK isoform specific binding partners have found in modulating kinase activity through direct interaction with catalytic domain or via altered cellular localization of kinases. ROCK inhibitors have been extensively used in studies using cancer cell line and rodent cancer models, and significant beneficial effect have been shown in many types of cancer.

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Evaluation of sodium glucose co-transporter 2 (SGLT2) inhibitors in cancer cachexia

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Abstract: Altered carbohydrate metabolism is one of the key feature of cancer cachexia. Tisdale [1] Sodium glucose co-transporter 2 inhibition to regulate blood glucose in diabetes mellitus in addition to their role in homeostasis, inflammation, cancer, lipid metabolism, cardio protective effects. The objective of present study was to evaluate role of Dapagliflozin and Empagliflozin in cancer cachexia in B16F1 cell induced cancer cachexia.B16F1 cells were cultured and injected in Balb/c mice by rapid hydrodynamic tail vein injection. Treatment was given for 4 weeks.Results showed beneficial effects of Dapagliflozin and Empagliflozin with respect to tumor markers, inflammatory markers, carbohydrate markers and prevented lipid breakdown. Empagliflozin restricted the skeletal muscle wasting but Dapagliflozin could not restrict skeletal muscle wasting. The systemic study of SGLT2 inhibitors suggests that SGLT2 inhibitors Dapagliflozin and Empagliflozin have potential in management of treatment of cancer cachexia.

KeyWords: SGLT2 inhibitors, Dapagliflozin, Empagliflozin, cancer cachexia

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Review on Regulatory Aspects of Nano-medicines

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Abstract: Nanotechnology is an emerging technology applied to the pharmaceutical sciences involving the development of Nano-medicines. Nano-medicines are advantageous over the conventional medicines as they provide target specificity and thus are highly useful in oncology. Wide range of application of Nano-medicines requires profound knowledge and characterization. [2] Their properties need to be extensively understood to avoid unpredicted effects on patients, such as potential immune reactivity. [2] The most significant concerns regarding the Nano-medicines are risk assessment, risk management and risk communication. [1] Although in-vivo animal experiments and ex-vivo laboratory analyses can increase our understanding of the interaction of Nano-medicines in biological systems, they cannot eliminate all the uncertainty surrounding the exposure of human subjects in clinical trials. [1] These safety concerns demand added stringency in the regulatory requirements and thus more involvement of regulatory agencies.

Since 1995, Nano-medicines are being used clinically and still they lack specific strategy for evaluating their safety, efficacy, compatibility, general protocol for pre-clinical development and characterization. [3]. It is moral responsibility of regulatory authorities' world-wide, to ensure safe and efficacious medicines for the patients. It is high time that various regulatory agencies worldwide, work together and frame regulations for the development and use of Nano-medicines, [3] giving emphasis on the ethical guidelines to balance benefit/risk ratio. This paper presents why different strategy to be adopted for Nano-medicines and the necessary steps to be taken for safe and effective administration of Nano-medicines to the patients.

Keywords: Nanotechnology, Nano-medicines, Oncology, Regulations

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BE A VEGETARIAN

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ABSTRACT: The word vegetarian comes from the latin word 'vegetus' that means 'lively'. There are several subdivisions which include Lacto-ovo Vegetarians, Lacto Vegetarians, Ovo Vegetarians, Pollo Vegetarians, Pesco Vegetarians and Vegans. According to Hinduism, benevolence in a man's heart is quite unlikely to indulge in deeds that may cause pain to other living beings so killing animals for feeding ourselves is not an option. Some people switch to vegetarianism due to concern over Health. Health Vegetarians can be divided into two groups: those who are primarily concerned with food additives, and those who are primarily concerned with the role of meat and animal fat in various degenerative diseases. Moreover Vegetarians have lower levels of certain risk factors for heart disease such as total serum cholesterol, triglycerides and low density lipo-proteins and the vegetarian diets seems to hold great promise as a major weapon in battle against morbidity as well as mortality from cardiovascular disease. Veganism is defined as a way of living that attempts to exclude all forms of animal exploitation and cruelty, whether for food, clothing or any other purpose.

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Role of tyrosine kinase receptor in type 2 diabetes

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ABSTRACT: Tyrosine kinases are important mediators of this signal transduction process, leading to cell proliferation, differentiation, migration, metabolism and programmed cell death. Tyrosine kinases are a family of enzymes, which catalyzes phosphorylation of tyrosine residues in target proteins using ATP. Tyrosine kinase inhibitors produces inhibition of the phosphorylation of target proteins by occupying the ATP-binding site of the tyrosine kinase. Tyrosine kinase inhibitors targets are c-abl, PDGFR, VEGFR2, EGFR. Tyrosine kinase leads to interaction of insulin with α subunit which leads to conformational change and activation of β subunit. This β subunit activation leads to phosphorylation of cellular protein substrates which leads to growth promoting effect and finally this phosphorylated and active substrate results in to insulin like effects. EGFR gives signaling activity of receptor and normal growth and it affects cell migration, proliferation, motility and apoptosis by ligand binding, trans-phosphorylation, ubiquitination that is protein degradation. C-abl is inactive in innate form and activate when interact with RFX1. Its inhibition results in reduced beta cell apoptosis, increased beta cell survival, and enhanced insulin production. Inhibition of PDGFR improves insulin sensitivity by promoting adipogenesis and adiponectin secretion, and suppresses inflammatory responses in islets. Thus, tyrosine kinase inhibitors can be potential target for type 2 diabetes.

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OPTICAL CHARACTERIZATION TECHNIQUES FOR NANOPARTICLES

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ABSTRACT: A nanoparticle is the basic and most useful component in the development of a nanostructure.It is science which basically deals with matter at the size or scale of 10^{-9} m = 1nm and it is also study of the deploying matter at molecular and atomic scales. It is far much smaller than the object that are showed or listed in the Newton's law of motion but larger than an atom or molecule that are coordinate by quantum mechanics.The properties of nanoparticles and nanomaterials differ meaningfully at nanoscale compared to macroscale (light visible). Nanotechnology includes all the variety of techniques for formulating, designing, characterizing and modifying the structures and materials. This study includes about the important basics of nanomaterials, trailed by a list of various commonly used characterization techniques. Vigorous techniques for characterization of nanomaterials are optical, electron probe, photon probe, ion particle probe and thermodynamics characterization techniques. The brief description ofoptical characterization techniques like Confocal scanning laser microscopy, scanning near field optical microscopy, two photon fluorescence microscopy, Dynamic light scattering and Brewster angle microscopy are well discussed together with its limitations and strengths. The careful selection of the technique for the characterization of nanomaterials play a vital role in success of the product.

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Biodegradable polymers: Properties and Application

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ABSTRACT: The amalgamation of polymer science and pharmaceutical science led to the introduction of polymers in the design and development of Drug Delivery Systems (DDS). There are many polymers available from the nature from which polymers don't show interaction with the Active Pharmaceutical Ingredient(API) , Amongst which Biodegradable Polymers are based upon drug delivery system has developed a promising clinical tool for specific targeting and controlled drug releasing delivery system . There are different delivery systems such as nanoparticles , microparticles , microencapsulation , etc for the drugs and its maximum absorption is necessary for the maximal effect of the drug. Delivery system should be such that it is both painless and effective along with minimal side effects . Polymers such as polyhydroxy alkenones (PHA) , polylactic (PLA) , polyester amid (PEA), etc. are used. These polymer are used as surgical sutures , wound dressing , tissue regeneration , controlled drug delivery system , gene delivery medical implants , etc .Various factors that affect these selection of biopolymer are drug release profile , degradation mechanism , toxicity profile , different routes of administration , etc . This suggest a revolution in the drug delivery system in pharma world . Its biodegradable nature , the compatibility , effectiveness and patient compliance can be an important factor that can be studied and focused upon.

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Regulatory Framework of Biosimilars in EU: Opportunities and Challenges

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ABSTRACT: A biosimilar is a biological medicine similar, but not identical, to an already registered reference bio therapeutic product in terms of quality, safety, and efficacy. Biosimilar medicinal products follow the specific provisions of EU legislation (the so-called "biosimilar pathway") which include defined high standards of quality, safety and efficacy. EU is the first in the world to set up legal framework and regulatory pathway for biosimilars. As mandated by law and in order to give guidance to industry, the EMA has developed overarching and product-class specific scientific guidelines on biosimilar medicines, thus providing a robust regulatory process to grant marketing authorizations for biosimilar medicinal products. This article deals with the evolution and current status of the regulation of biosimilars in EU and highlights the challenges and future prospects. The EU regulatory system for biosimilars is complicated in the way that, marketing authorization is handled centrally and matters of interchangeability and substitution is handled by the member states. Although biosimilar products have been registered and approved for use in the EU for more than a decade, there is increasing speculation and excitement on the potential for biosimilars with increasingly complex structures. With great achievements come greater challenges for maintaining diligence and patient safety with currently approved products and registering biosimilars with increasing complexity. For better understanding and broader perspective of biosimilars regulations in EU we will carry out strength, weakness, opportunities and challenges analysis.

Keywords: Biological, Biosimilar, EMA (European Medical Agency), Marketing authorization, Interchangeability, Substitution.

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SCREENING AND SELECTION OF COFORMER FOR LUCRATIVE COCRYSTAL FORMATION

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ABSTRACT: In the determination of the efficacy as well as the activity of a drug, the solubility and their dissolution rate play important roles. Many of the drug molecules that are discovered have limited application due to their poor solubility and dissolution profiles. The significant challenge for a successful formulation development in pharmaceutical industries is to improve the solubility and dissolution of poorly water soluble drugs without altering their molecular structure.Cocrystallization offers the all above advances required for solubility and bioavailability enhancement. In the manufacturing of cocrystal selection of coformer is crucial step. Selection of proper coformer abstain the excess cost of manufacturing of cocrystal.

In the present review various methods for screening and selection of coformers are described, which may implemented for selection for best suitable coformer for lucrative cocrystal formulation. The different theoretical and analytical parameters like PKa rule, Hansen Solubility parameter, Thermal analysis, synthon Engineering approach are discussed in present review.

Key words: cocrystallization, coformer, PKa rule, Hansen solubility parameter, Thermal analysis.

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PHARMACOVIGILANCE REGULATORY FRAMEWORK OF INDIA, SOUTH KOREA AND CHINA

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ABSTRACT: The global pharmacovigilance(PV) market size was estimated at USD 4.31 billion in 2018 .The aim of PV is to enhance patient care and patient safety in relation to the use of medicines; and to support public health programmes by providing reliable, balanced information for the effective assessment of the risk-benefit profile of medicines. Asia's pharmaceutical market is generally dominated by generic drugs, the biggest players being China and India. The volume of clinical trials being conducted in the Asian countries has been growing rapidly in recent years as emerging markets grow thus stressing on the need of more progressive PV regulations. In India, the IPC-PvPI is a WHO Collaborating Centre for Pharmacovigilance in Public Health Programmes and Regulatory Services and the culture of reporting of ADRs has achieved remarkable success, with 250 PvPI-established adverse drug monitoring centers all over India and provision of training to healthcare professionals. South Korea has excellent infrastructure such as broad distribution of electronic medical recording systems and a nationwide single healthcare insurance as a Pharmacovigilance System and has the highest rate of ADR reporting among Asian countries. As per the Uppsala Monitoring Centre's data 2017-18 China has a different (other than ICH-E2B) international standard form for transmission of Individual Case Safety Report (ICSR). In December 2015, the China Food and Drug Administration (CFDA) proposed a number of revisions that would modify existing rules regarding medical device adverse event reporting. Further this proposal will deal with real world evidence and current regulatory framework in India, South Korea and China.

Keywords: Pharmacovigilance, regulations, India, South Korea, ICH-E2B

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Nanopreparations for mitochondria targeting drug deliverysystem

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Abstract: Mitochondria are a novel and promising therapeutic target for diagnosis, treatment and prevention a lot of human diseases such as cancer, metabolic diseases and neurodegenerative disease. Owing to the mitochondrial special bilayer structure and highly negative potential nature, therapeutic molecules have multiple difficulties in reaching mitochondria. To overcome multiple barriers for targeting mitochondria, the researchers developed various pharmaceutical preparations such as liposomes, polymeric nanoparticles and inorganic nanoparticles modified by mitochondriotropic moieties like dequalinium (DQA), triphenylphosphonium (TPP), mitochondrial penetrating peptides (MPPs) and mitochondrial protein import machinery that allow specific targeting. The targeted formulations exhibited enhanced pharmacological effect and better therapeutic effect than their untargeted counterpart both in vitro and in vivo. Nanocarriers may be used for bio-therapeutic delivery into specific mitochondria that possess a great potential treatment of mitochondria related diseases. In this poster, I will summarize five main mitochondrial targeting strategies and some nanopreparations made for targeting mitochondria to cure diseases.

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4-SUBSTITUTED COUMARIN AS ANTICANCER AGENT, A REVIEW

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ABSTRACT: Coumarins are the oxygen containing fused heterocyclic which is known as benzopyrone class. They are the naturally occurring compounds comprising of benzene and α-pyrone rings. When coumarins are substituted at C_4 position, it gives significant pharmacological activities such as anti-inflammatory, antidepressant, antitumor, antimicrobial, antiviral, anticoagulant, antioxidant and many more. According to world health organisation cancer is the second leading cause of death globally and is estimated to account for 9.6 million deaths in 2018. Substitution at C_4 position of coumarin shows cytotoxic activity in many cancer cell lines and targets many pathways in cancer: kinase inhibition, cell cycle arrest, telomerase inhibition, anti-proliferative activity, tubulin polymerase inhibition, inhibition of 5-lipoxygenase metabolic pathway and many more. So far, many 4-substituted coumarins have been investigated as anticancer agents as it shows potent and broad spectrum in-vitro cytotoxic activities and it is expected to discover more novel 4-substituted coumarin. The present compilation discusses the progression of C_4 substituted coumarin as anticancer agents.

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ELECTROSPINNING OF NANOFIBERS AND THEIR APPLICATIONS

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Abstract: Electrospinning is a useful and efficient technique to produce ultrafine polymeric fibers. It has been a process of great scientific and industrial interest due to its versatility, cost efficiency and potential to be used in a wide range of applications, resulting in an outstanding potential for nanotechnology research. As it is regarded as the most promising approach to produce continuous nanofibers on a large scale, a huge amount of work and study is observed to be carried out in this area both in academic and industrial circles, aiming to utilize the technology in a wide range of applications. The technique has been used with many synthetic and natural polymers. This poster on electrospinning gives detailed information on history of electrospinning, process theory and basic principles, parameters that influence the process and fiber morphology, advantages of superior properties and applications of electrospun nanofibers.

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Recent Advances in the Discovery of Small Molecule EGFR Inhibitors

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Abstract: Lung cancer is one of the leading cancers worldwide and accounted for 2.09 million cases in 2018. Epidermal growth factor receptor (EGFR) is one of the most commonly altered genes in human cancer by way of overexpression, amplification, and mutation.First, second and third generation EGFR inhibitors are molecular targeted therapy of EGFR-mutant NSCLC patients. First generation of EGFR tyrosine kinase inhibitor (Gefitinib, Erlotinib, Icotinib) were effective for the EGFR mutant first liner NSCLC but resistance was seen due to point mutation of T790M. Second generation (Afatinib, Dacomotinib) were irreversible EGFR inhibitors that bind to Cys797 and was seen in preclinical experiments to effectively inhibit EGFR with activating mutations as well as those with the T790M resistance mutation but have narrow therapeutic window toxicity liabilities. Third generationEGFR inhibitors were recently (Osimetinib, rociletinib, Olmutinib, nazartinib) developed to target mutant EGFR. This class of inhibitor also binds covalently to Cys797, and largely spares WT EGFR, thereby decreasing toxicity and permitting the use of doses that fully suppress T790M. This present review is mainly focusing on recent development in the research and discovery of third generation inhibitors with the hope that this will be useful for discovery of future EGFR inhibitors coming to the clinical stage.

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Current Regulatory Authority Actions against Misbranded and Adulterated Drugs in India

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Abstract: An adulteration is the substance within food and drugs which chemically weakens the quality and effectiveness of the drug. Worldwide every nation is the victim of misbranded and adulterated drugs, which are responsible for life threatening issues, financial loss of consumer and manufacturer and loss in trust on health system. For minimizing adulterated and misbranding drugs or not of standard quality drugs, there is animmediate requirement of firm regulation and legal action against theadulterated drugs. At present every country has taken some preventive steps for their nation to fight against poor quality of drugs.The substitution of crude drug is an intense problem. Replacement is useful in such areas where unavailability of specific crude drug or undesired adverse effects of desired crude drug are there and have a choice of other drug with similar pharmacological effect and less unwanted adverse effects. But most of the time, it is insufferable because the transformation of authentic drug into substandard drug may develop variety of unwanted adverse effects from mild and moderate to severe life threatening reactions. So, understanding of all the ways of adulteration and substitution is essential to correct this illegal act and increase consumer's safety. Nevertheless, India has taken some preventive steps in the country to overcome against the poor quality of drugs for securing and encouraging the public health. For betterment for the public health various guidelines have been created for stopping the adulteration which monitors the quality of the crude drugs. (Kumar et al.)[1]

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CRISPRi/CAS9 BASED DESIGNING OF sgRNA FOR SUPPRESSION OF sgt1 GENE IN POTATO

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ABSTRACT: Potato is staple non grain crop which is used as food in eachand everyhouse in different forms. A part of Solanaceae family it produces α-solanine as a secondary metabolite.Formation of glycoalkaloids and its toxicity become an important focus for researchers and public health agencies because its high demand and consumption. Research suggested that susceptibility of humans to α-solanine poisoning are high and very variable; oral doses in the range of 1 to 5 mg/kgbody weight are marginally to sever toxic, whereas 3-6 mg/kg body weight can be lethal. In genome editing CRISPRi/Cas9 is a latest technology which has high efficiency and molecular targeting with less off-target effects. With the help of CRISPRi/Cas9 technology suppression of sgt1 gene codes for UDP-galactosyl transferase enzyme that adds sugar moieties to the Solanidine residue and convert it in the α-solanine.In CRISPRi/Cas9 technology gRNA is an important complementary sequence of target sequence which guides Cas9 protein for the modification of targeted gene. The present study discusses about designing of sgRNA for suppression of α-solanine level.

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Role of Anti-diabetic agent in modulation of depressive-like behavior comorbid with glucose intolerance: Activation of AMPK

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ABSTRACT: Background: Diabetes, a systemic metabolic brain state doubles the risk of the depressive like behavior.

Aim and objective: Our main objective of the study was to evaluate anti-diabetic drugs for treatment of diabetes associated depression.

Material and Methods: Empagliflozin was evaluated for diabetes associated depression in *in-vitro* model of zebrafish and in *in-vivo* study on C57BL/6 mice using unpredictable chronic mild stress model. The treatment was given for 4 weeks and behavioral and biochemical parameters were evaluated. Latterly, animals were sacrificed and brain samples were isolated for determination of neurotransmitters like serotonin and dopamine, enzyme activity for AchE, MAO-A, MAO-B, aldose reductase and histopathological evaluation. Immunohistochemistry, gene expression and cell apoptosis by TUNEL assay was carried out.

Results: The result showed that empagliflozin reversed the effect of depressive behavior in zebra fish, indicated by behavioral parameter in T and Y maze and forced swim and tail suspension test suggests that empagliflozin ameliorates the depressive behavior. The biochemical parameters like glucose, lipids, and CRP and LDH levels were significantly improved with the treatment. Upon the treatment, serotonin level was significantly increased where dopamine was down regulated and unchanged. Treatment showed potent anti oxidant and anti stress activity on depressive animals. Histopathology, immunohistochemistry and TUNEL assay outcomes claimed neuroprotection from brain injury in neuronal cells and astrocytes upon treatment groups. Gene expression studies of AMPK, IL-6, CNTF, MMP-9 and caspase 3 evident the anti depression activity of empaglifozin by activation of AMPK pathway.

Keywords: AMPK-Pathway, Diabetes, Depression, Empaglifozin, Tunnel-Assay

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Development and validation of stability indicating RP-HPLC method for simultaneous determination of Abacavir sulphate and Lamuvidin in tablet dosage form and forced degradation study by QbD approach

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ABSTRACT: A simple, precise and rapid stability indicating RP-HPLC method has been developed for the simultaneous estimation of Abacavir sulphate and Lamuvidin in Pharmaceutical dosage form in presence of degradation products. It involved Inertsil ODS C_{18} column with dimensions 250mm x 4.6mm with particle size of 5µm. The separation was achieved using the mobile phase A consisted of mixture of ammonium acetate buffer and methanol -50:50(%v/v) Mobile phase at flow rate of 1.0 ml/min. The effluent is monitored at 282 nm. The retention time of Abacavir sulphate and Lamuvidin was found to be 6.273 and3.258, respectively. By applying QbD approach two active compounds and their degradation products were separated and the optimized method was applied for forced degradation study. Various factors affecting the method were optimized using a d-optimal design. Point verification of actual versus optimized predicted trials was performed. A Design space in which the method was robust could be generated successfully. Acid, alkali, and Peroxide degradation was carried out and significant degradation product was achieved .The method was found to be specific enough to separate degradation products from main analytes. The method was linear in the range of 30-90 µg/ml (R^2=0.999) and 30-70 µg/ml (R^2=0.999) for Abacavir sulphate and Lamuvidin, respectively. The described method was validated with respect to system suitability, specificity, linearity, accuracy, precision and robustness. Result of each parameter was met with its acceptance criteria.

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P-104

Enhancement in Transdermal Permeation of Lipophilic Drug by Preparing Nanoemulgel

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ABSTRACT: The Nano emulsion-based gel is one of the approaches to enhance the systemic delivery of lipophilic drugs. Nanoemulgel is a combined approach of two different systems emulsion and gel. This fusion of two different dosage form advantageous in some ways. Mostly the lipophilic drugs can easily incorporate into the oil phase of emulsion and thus its permeability may enhance several folds due to the wide distribution of drug in oil phase. That will result in increased pharmacokinetic and pharmacodynamic profile of drug. While gel base provides hydrating effect on skin; that will also improve the permeability. This system is basically oil in water (o/w) type of emulsion gel. That is non greasy, better user compliance and produce more stable emulsion by decreasing surface as well as interfacial tension. Emulsion based gel is widely used in food industry and as well as cosmetic industry. It is able to produce controlled release as well as sustain release of drug throughout the skin. Various type of fatty acids and vegetable oils shall be use in preparation of emulsion. In addition to this synthetic or semisynthetic oil also can use which will improve the drug loading.Different type of gelling agent shall be used that will create interconnecting network structure in continuous phase. Due to this interconnecting network stability of nano emulsion also increased.

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P-105

21st CENTURY CURES ACT

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ABSTRACT: 21st Century Cures Act, was signed into law by President Obama on December 13, 2016. Enacted by the 114th Congress with bipartisan support, the "Act to Accelerate the Discovery, Development, and Delivery of 21st Century Cures, and for Other Purposes," (Public Law 114–255) also known as the 21st Century Cures Act was issued. The 311-page bill is composed of 3 divisions (21st Century Cures, Helping Families in Mental Health Crisis, and Increasing Choice, Access, and Quality in Health Care for Americans), 18 titles, and 23 subtitles. Some of the portions addresses specific public health concerns such as mental health, the opioid crisis, and vaccine development, but major segment focuses on research, drug and device development, and associated regulatory issues. Cures enhances our ability to modernize clinical trial designs and clinical outcome assessments, which will speed the development and review of novel medical products, including medical countermeasures. It aids FDA improve ability to recruit and retain scientific, technical and professional experts and also establishes new expedited product development programs. Furthermore, the Cures Act also intends FDA to create one or more intercenter institutes to help coordinate activities in major disease areas between the drug, biologics and device centers and improves the regulation of combination products.

Keywords: Product development, Work plan, Funding, Statutory requirement.

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P-106

Mellitus and Alzheimer's Disease: Bridging pathophysiology

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ABSTRACT: Diabetes Mellitus (DM) and Alzheimer's Disease (AD) are two most devastating and incurable diseases found in the most old age population. These two prevalent diseases develop mostly among geriatrics population of age 65 and above. Numerous epidemiological, pathological and clinical affirmation has confirmed the co-existence of these two diseases. There has been assuring progress in the recognition of the pathological linkage between t2DM and AD. As per t2DM common pathological mechanism like central nervous system insulin resistance, oxidative stress and inflammatory response would increase the risk of AD in diabetic patient. It is concluded that anti-diabetic medicines can be effective to improve dementia in early stages of AD.The aim of this poster is to understand the possible theories about the interplaying risk factors and pathophysiological linkage.

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Mechanochemistry as a sustainable technique for the synthesis of drugs

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Abstract: Solvents constitute one of the major economic costs and environmental impacts of the pharmaceutical industry. To mitigate this impact, many sustainable strategies using the green chemistry approach have been sought for. Mechanochemistry is one such promising technique towards the 'nosolvent' approach in the synthesis of drugs. It is the amalgamation of chemistry and mechanical engineering by using ball mills. (Avila-Ortiz et al. [1])And from the pharmaceutical perspective, it can be used to synthesise chemical moieties without the use of solvents or induction of thermal conditions. It works on the principle of induction of chemical process by absorption of mechanical energy.(Howard, Cao, & Browne. [3])This method offers increased efficacy, selectivity and reduction in reaction time. Mechanochemical reactions have found their applications in synthesising small organic molecules and most commonlyhydrazones. This poster presents the potential of mechanochemistry in the synthesis of hydantoins(Konnert et al. [4])and hydantoin-based drugs such as nitrofurantoin anddantrolene.These are the most commonly used anti-epileptic, anti-bacterial and myorelaxant drugs.(Colacino et al. [2])And by employing mechanochemistry the frequent use of solvents which are otherwise used to synthesise these drugs can be curbed. Furthermore, the potential of this method in developing various other drugs has been reviewed and discussed.

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P-108

New molecular insights into dual inhibitors of tankyrase as Wnt signalling antagonists: 3D-QSAR Studies on 4*H*-1,2,4-triazole derivatives for design ofnovel anticancer agents

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ABSTRACT: Genetic mutations in APC or CNTBB1 gene with aberrant canonical Wnt/β-catenin pathway are responsible for more than 90% of colorectal carcinogenesis.Tankyrases (TNKSi) are known to down regulate Wnt signaling by stabilizing AXIN protein through poly(ADP ribose)polymerization or PARSylation process and subsequently, promoting degradation of intracellular β-catenin. Tankyrase enzymes are modulated by range of known inhibitors which bind individually to any of thenicotinamide or induced adenosine pockets or as dual binding antagonists.Hence, for designing of dual tankyrase inhibitors as Wnt signaling antagonist; we carried out 3D-QSAR studies using data set of 51 molecules of reported 3,4,5-trisubstituted 1,2,4-triazole derivatives. These reported 51 molecules were divided into training set (39 molecules) and test set (12 molecules), aligned and subjected to generate CoMFA, CoMSIA and HQSAR models. CoMFA analysis showed q^2value of 0.694, r^2_{ncv} value of 0.991 and r^2_{pred} value of 0.641. Optimized CoMSIA analysis (SEHA) showed q^2 value of 0.624, r^2_{ncv} value of 0.909 and r^2_{pred} value of 0.850. HQSAR analysis showed q^2, $r^2$and r^2_{pred} values of 0.781, 0.901 and 0.811, respectively. Contour maps from all studies provided significant results with identification of desired spatial arrangement of different atoms or functional groups in a molecule. Triazole ring system-based molecules were reported as potent tankyrase inhibitors. These noteworthy results were employed for the design of different triazolederivatives as potent tankyrase inhibitors, wherein series of twenty different molecules are designed for evaluation of their potential as novel tankyrase inhibitors.

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Self Nano-Emulsifying Drug Delivery Systems (SNEDDS) of Ezetimibe for Enhancement of Oral Bioavailability

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ABSTRACT: The objective of present study is to develop a Lipidicoral formulation i.e. Self-nanoemulsifying drug delivery systems (SNEDDS) of ezetimibewith aim to increase its bioavailability in comparison with marketed product. Bandyopadhyay et al. [1] describeabouezetimibe which belongs to BCS class II drug, it havingpoor water solubility(0.00846 mg/mL) and good permeability (Log p 4.56). It is not only act as anti-hyperlipidemic drug, but also has potential as cholesterol inhibitor for familial hypercholesterolemia, hepatic steatosis and gallstone diseases.Long chain and medium chain triglycerides are reported to decrease first pass metabolism and to increase bioavailability.Ternary phase diagrams are to be prepared for specific concentration of lipids, surfactants and cosurfactants. The optimized formulation will be solidify using suitable adsorbance if required. Bioavailability studies will be done in suitable animal model and compared with selected marketed product. Self-emulsifying dosage forms potential is proven by success full marketed products like Sandimmune®.

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P-110

Current Regulation of Drug Eluting Cardiac Stent in USA, EU & India

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Abstract: Medical devices are a global industry with continuous growth because of advancements in technology and new innovation. Now a days there is increase in cardiac disease amongst the population. As there is high level of stress, the disease such as Angina, cardiac arrest, heart failure are most prevalent. Even young population are suffering from cardiac diseases.Hence new interventions and treatments are coming up and one such intervention already in market is 'Drug Eluting Cardiac Stent.' The drug eluting stent (DES) is the combination of Drug and medical device where together they provide primary mode of action to prevent restenosis.Moreover due to Increase in prevalence of cardiovascular diseases, rising aging population & growing acceptance for minimally invasive endovascular surgeries, there is the growth of the Drug Eluting Stent in the market.Hence it becomes important to know about its regulations.

P-111

Microfluidic Devices for Detection of Cancer

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Abstract: More than two decades ago, microfluidics began to show its impact in biological research. Since then, the field of microfluidics has evolving rapidly due to its high sensitivity, high throughput, less material consumption, low cost, etc. Microfluidics holds great promise in cancer diagnosis and also serves as an emerging tool for understanding cancer biology. Currently, expensive, complex and invasive procedures, such as surgical tissue biopsies, are used for cancer screening. Advancements in microfluidics and lab-on-a-chip approaches have been made to develop minimally invasive and miniaturized platforms to identify and segregate circulating cancer biomarkers such as exosomes, circulating tumour cells (CTCs) and cell-free DNA (cf-DNA) from body fluids. Microfluidic based platforms are portable and can be easily designed for point-of-care diagnostics. Developing and applying the state of art microfluidic technologies to address the unmet challenges in cancer can expand the horizons of not only fundamental biology but also the management of disease and patient care. Despite the various microfluidic technologies available in the field, few have been tested clinically, which can be attributed to the various challenges existing in bridging the gap between the emerging technology and real-world applications. This presentation reviewed role of microfluids in cancer research, including the history, recent advances, existing and potential applications of microfluidic technologies in detection of cancer biomarkers.

Key words: microfluidics devices, cancer, bio-markers.

P-112

AN EMERGING THERAPY OF FUNGAL INFECTION

RAJ PACHANI

Abstract: Fungal infections of the skin are one of the often faced with dermatological diseases in worldwide. Topical therapy is an attractive choice for the treatment of the cutaneous infections due to its advantageous such as targeting of drugs to the site of infection and reduction of the risk of systemic side effects. Currently, antifungal drugs are generally used as conventional cream and gel preparations in topical treatment. The efficiency of that treatment depends on the penetra- tion of drugs through the target layers of the skin at the effective concentrations. However, stratum corneum, the out-ermost layer of the skin, is an effective barrier for penetration of drugs into deeper layers of the skin. The physico-chemical characteristics of drug molecules and the types of the formulations are effective factors in topical drug delivery. This poster is comes up with the new alternative therapy of fungal infection by the Solid-Lipid Nano Carriers(SLN) because this drug delivery has unique characteristics which fulfill all the requirements of drug delivery for fungal infection by topical rout.

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Recent Progress in the Development of Anaplastic Lymphoma Kinase (ALK) Inhibitorsas Anti-Cancer Agents

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Abstract: Cancer is the most widespread and feared disease among which lung cancer is most prevalent and accounted for 1.76 million deaths all around the globe in 2018 [1]. Anaplastic lymphoma kinase (ALK) is a membrane-spanning receptor tyrosine kinasebelonging to insulin receptor superfamily. It was first identified as nucleophosmin (NPM)-ALK fusion protein in anaplastic large-cell lymphoma (ALCL)[2].Subsequently, more than two dozens of ALK-Fusion proteins and ALK mutation have been reported in a number of other lymphomas, especially in non-small cell lung cancer (NSCLC) [3]. Rearrangements in ALK gene have been proven to contribute to tumor formation & maintenance [4].Due to its implied therapeutic opportunities, it has become one of the most studied targets in treatment of various cancers, especially NSCLC and ALCL. Different therapeutic approaches targeting the ALK pathway are under development and Crizotinib, Ceritinib, Alectinib, Brigatinib and Lorlatinib are clinically available for ALK-positive cancer.However, the emergence of aberrant mutations and drug resistance led to the development of the first-, second-, third- and fourth-generation ALK inhibitors [5].Herein, we describe signaling pathways of ALK as well as enlist drugs under development with their efficacy forthe treatment of ALK positive NSCLC.

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Small Molecule Inhibitors Targeting Cyclin-Dependent Kinases in Human Cancers

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Abstract: The Cyclin-dependent kinase (CDK) family is among the most investigated protein serine/threonine kinase groups owing to its general role in regulation of the cell cycle and in oncogenesis. They along with their associated cyclins modulate the transcription activity. There are around 21 known CDKs that can interact with 29 cyclins among them three (CDK1, 4 and 5) are involved in cell cycle, and five (CDK 7, 8, 9 and 11) are associated with transcription. While multiple deregulations of CDKs is associated with tumor development. Thus, CDKs is regarded as a promising target for cancer drug development. Till date, three different generations of CDKs inhibitors have been developed. The first-generation CDK inhibitors (pan-CDK inhibitors) were suffered from too high toxicity. The Second-generation CDK inhibitors (e.g. Dinaciclib) were designed to be more specific for CDK1 and 2 or to be generally more potent inhibitors. Again, the development of second-generation inhibitors was discontinued due to high toxicity liabilities. The third-generation inhibitors (selective CDK4/6 inhibitors; e.g. Palbociclib, Ribociclib and Abemaciclib;) is the most interesting and promising class of CDK inhibitors identified due to their high *in-vivo* efficacy and limited toxicity issues. The review is an effort to summarize recent advancements in medicinal chemistry aspects of small molecule CDK inhibitors as promising anti-cancer agents which would certainly help researchers to bring further developments of small molecule CDK inhibitors.

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The Influence of Nutrimiromics on Inflammation and other various Chronic diseases.

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Abstract: Nutrimiromics involves the study of the micro-RNAs(mi-RNAs) that are responsible for causing inflammation as well as the chronic diseases such as hypertension, diabetes(type 2), cardiovascular diseases and cancer.Coinetti C. et al[1]. The micro-RNAs (mi-RNAs) regulates the expression of the genes physiologically as well as pathologically and they act by silencing the gene responsible for mRNA degradation or repression by binding to a specific target messenger RNA(mRNA) Huntzinger E., Izaurralde E. et al [2]. The functions of nutrimiromics can be controlled by environmental factors as well as by dietary factors, thus giving an idea that dietary changes can lead to lower the risk of development of chronic diseases in the future Vrijens K., Bollati V., Nawrot T.S. et al [3],Tili E., Michaille J.-J., et al [4], Vinciguerra M., Sgroi A. et al [5], Ortega F.J., Cardona-Alvarado M.I., et al [6]. Also it was observed that certain minerals, vitamins and nutrients could be responsible for change in mRNA concentrations thus controlling gene expression indirectly Zhang L., Hou D.,et al [7].

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P-116

Regulatory account on Generic drug registration and inter comparison in CIS Countries.

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Abstract: Generic drug registration in CIS countries through common technical documents. In the Cis region it is have a Country specific guideline. In this CIS countries registration it also include various policies like a drug pricing policy, national health policy and many more policy. Generic drug registration main requirement for that is the technical document and in that various modules in the common technical document. In the CIS countries comparison in mainly focus on chemistry, manufacturing and control which is comes under the quality parts. Second comparison is product administrative information which is comes under module 1. So there is a given detail about the comparison and various policy and regulation.

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Medical device regulations in Europe and China

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Abstract: Medical Device is an emerging market in last twenty years since the use of medical device is increase rapidly throughout theglobe. Number of patients around globe depend on medical device for the diagnosis &management of diseases. Regulation of the medical device differs within the nation are based on their own Regulatory bodies. In order to market any medical device, marketing authorization from regulatory authority is required. The process of obtaining authorization is compound, multistep and requires review of information by proficient authorities. Upon examining the information provided by manufacturer, marketing authorization is permitted by the Regulatory authority. In EU, national authorities give approval for marketing medical devices. A system of third party compliance is there, where Notified Bodies (Third Party) ensure quality assurance, pre and post approval.The European Union is responsible for the proposing and implementation of new regulations in EU, the European commission put first medical device directive into the place in 1993 under the council directive 93/42/EC, which is the first attempt to harmonize the medical device regulation which is marketed across EU member states. (R Sethi et al.)[1]Medical device regulations around world have remarkable variations. The Chinese medical device market, like China's economy, is growing quickly.The National Medical Products Administration (NMPA), previously the China Food and Drug Administration (CFDA), is the institution responsible for pharmaceuticals and medical devices regulations in China.Advantage of harmonizing regulations also reviewed.(R Liu.) [2]

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Recent Developments in Intracellular Organelle Targeted Delivery Using Nanoformulations

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Abstract: Nanoparticles as well as nanocarriers have witnessed a rise in usage & in research owing to an increased demand & necessity of targeted drug delivery to provide a localized therapeutic effect while minimizing the adverse effects, hence facilitating the development of safer medicines. [1]Numerous nanocarriers have been developed which can effectively deliver various drugs to intracelluar matrix as well having the ability to target specific intracellular organelles.Recent advances in ligands for intracellular delivery includes cell-penetrating peptides (CPPs), nuclear localization signals (NLS), mitochondrial localization signal, ER signal peptide & other non-peptide ligands have paved a way forward for targeted delivery to the nucleus, cytosol, mitochondria& the lysosomal complex. [3] Liposomes remain the most common form of nanocarriers which are modified to achieve targeted & specific delivery to the above organelles. [3]Herein, we describe various nanocarrierswith the organelles they target which are undergoing extensive research for intracelluar delivery, their advantages, future prospects in their development as well as their potential & radical utility in improving & enhancing treatment of a number of diseases & conditions.

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CoMFA and CoMSIA Studies on 2-Methoxyacylhydrazone Derivatives as Phosphodiesterase 10A Inhibitors

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Abstract: Schizophrenia is a chronic disorder which affects the person's ability to think, feel and behave clearly. According to the WHO, 21 million people are currently suffering from this disease. The phosphodiesterase 10A (PDE10A) isregarded as a potential target for schizophrenia. PDE10A inhibitors are effective against the negative symptoms of schizophreniain contrast to the current drugs available for therapy. In this study, 3D-Quantitative Structure Activity Relationship (3D-QSAR) studies were carried out on a series of 2-methoxyacylhydrazone analoguesto find out the correlation between structure and function using the chemometric technique. For the 3D-QSAR studies, two models were generated using CoMFA and CoMSIA in SYBYL X. The statistical qualities of generated models were justified by internal and external validation, i.e., cross-validated correlation coefficient (q^2), non-cross-validated correlation coefficient (r^2_{ncv}) and predicted correlation coefficient (r^2_{pred}), respectively. The optimal CoMFA and CoMSIA models yielded a leave-one-out correlation coefficient (q^2) of 0.585 and 0.649, respectively. 3D contour maps generated from CoMFA and CoMSIA have identified several key features responsible for the inhibition activity. The obtained results can be served as a useful guideline for designing novel 2-methoxyacylhydrazone analogues with improved inhibitory activity against PDE10A.

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A Practical Approach: bridging of pharma projects designing and establishment with the regulatory requirements as per Current Indian regulations

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ABSTRACT: The pharmaceutical sector was valued at US$ 33 billion in 2017. The country's pharmaceutical industry is expected to expand at a CAGR of 22.4 per cent over 2015–20 to reach US$ 55 billion. India's pharmaceutical exports stood at US$ 17.27 billion in FY18 and have reached US$ 19.14 billion in FY19. Pharmaceutical exports include bulk drugs, intermediates, drug formulations, biologicals, Ayush & herbal products and surgicals.Nowadays regulations are becoming stringent and warning letters are increasing day by day because of rules and regulations. Main reason for increasing in warning letters because of regulatory affairs authorities are looking for safety and efficacy very precisely. Rules and regulations are improvised for safety of the patients. Regulators plays a major role in the safety and efficacy of the patients. Pharmaceutical company must be well designed, developed according to the rules and regulations given by the government. Problems related to the manufacturing premises is the main cause for the warning letters nowadays. Manufacturing premises must be properly designed so the drug that are manufactured in accordance with the regulation. Proper knowledge about the pharmaceutical formulations should be known. Manufacturing details according to the current Indian regulations.

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Liposomal Drug Delivery for Tumor Targeting

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Abstract: Liposomes as nanocarriersare an emerging area for targeting a tumor site, intracellular delivery, organelle-specific targeting and triggered release of therapeutic payloads.The use of nanocarriers in cancer therapy poses several advantages, including increased drug accumulation in desired target tissues and absence of harmful effects. These nanosized, lipid bilayered vesicles have become popular as drug delivery systems owing to their efficiency, biocompatibility, enhanced solubility of chemotherapeutic agents and their ability to encapsulate a wide array of drugs. Liposomal drug delivery systems improve the pharmacokinetic and pharmacodynamic profiles of the therapeutic payload, promotecontrolled and sustained release of drugs and exhibit lower systemic toxicity compared with the free drug. Passive and ligand-mediated active targeting promotes tumor specificity with diminished adverse effect. Recent advances in liposomes for targeting tumor delivery include Cancer cell receptor, tumor microenvironment, local stimuli strategies like pH, temperature, enzyme triggered drug delivery. Recent efforts have concentrated on the development of multifunctional liposomes that target cells and cellular organelles with a single delivery system. Here, we discuss the recent advances in liposome research in tumor targeting.

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Nutraceuticals Guidelines and Regulations in USA, JAPAN And INDIA

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Abstract: A Nutraceutical is defined as any substance that may be considered a food or part of a food and provides medical or health benefits including the prevention and treatment of disease Pharmaceutical and nutritional companies are aware of the monetary success taking advantage of the nutraceuticals and dietary supplements. Worldwide regulatory authorities are focusing on the Product Quality and Safety as these products are meant for human consumption. As Nutraceutical products are reaching from one country to another, maintaining safety and quality standards as per various regulatory guidelines set by the respective governments becomes important; which can be a real driver for the industry growth. Foods and food habits in today's lifestyle have lead to the disturbances in an ideally nutritionally balanced body. Therefore in such state if "food be your medicine" then it would be great to achieve a healthy body and mind. But now it is clearly understood that the regulations for clinical evidence and safety of such products cannot be less stringent than rules for modern medicines and thus the science of nutraceutical is progressing. The global nutraceutical market will reach $285.0 billion by 2021 from $198.7 billion in 2016 at CAGR of 7.5% from 2016-2021. This poster provides a review of the Nutraceuticals regulations set out by US Food & Drug administration in USA and in Japan by Pharmaceuticals and Medical Devices Agency and in India by Food Safety Standard Authority of India.

Keywords: Guidelines of Nutraceuticals,Regulations, USFDA, FSSAI, PMDA, Market Scenario

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Role of Arf in Lung Cancer

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Abstract: Who reportslung cancer to top the list when it comes to the increasing rates of mortality and incidence due to its poor prognosis. There are majorly two types of lung cancers, small cell lung cancer (sclc) and non-small cell lung cancer (nsclc) consisting of adenocarcinoma, squamous cell carcinoma and large cell carcinomas. Arf which is also known as $p14^{arf}$ in humans and $p19^{arf}$ in mouse is a nucleolar protein and a member of ink4, a family of cyclin-independent kinase inhibitors (ckis). These genes are encoded within cdkn2a locus on chromosome number 9p21. The role of $p14^{arf}$ has been documented as a potential target for nsclc. $P14^{arf}$ has a basic mechanism of inhibiting the mdm2(mouse double minute 2) protein which exhibits inhibitory action on p53, a tumor suppressor phosphoprotein, thus playing a role in various tumor suppression activities such as growth inhibition, dna damage, autophagy, apoptosis, cell cycle arrest, etc. The main focus of this review will be to incorporate different mechanisms through which the arfs can target lung tumor suppression. This review summarizes the available data, based on the molecular mechanisms and their related signalling pathways, to show how $p14^{arf}$ functions in different types of lung cancer.

Keywords: lung cancer, NSCLC, Arf, tumor supression, DNA damage, autophagy.

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Nanosuspension: A novel approach for poorly water soluble drug

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Abstract: Most of the investigational and new drugs have poor physicochemical properties due to shifting of drug development approach from trial and error based to computer aided drug design. Various approaches are used to formulate drug delivery systems for such poorly soluble drugs like nanosuspension,microspheres, solid nanoparticles,liposomes,niosomes,nanocrystals,nanocapsules etc.(1) Almost all, nanosuspension technology is preferred when drug have poor solubility, low log P, high melting point and high dose. Nanosuspension is colloidal biphasic dispersion system in which nano sized drug particles are suspended into aqueous vehicle stabilized by surfactant.The major advantage of this technique is simplicity, scalability and applicability to most of the drugs(2). There are main two process technologies to produce nanosuspension namely top down and bottom up process. Top down technology include methods like High Pressure homogenization, Media milling,Nanoedge.Bottom Up technology include methods like Solvent-antisolvent,Supercritical fluid, Emulsification solvent evaporation.Nanosuspensioncan be administered by various routes like oral,parenteral, pulmonary and additionally for drug targeting and site specific drug delivery(3). Thus we can conclude that nanosuspension can be a suitable approach to delivery drug over the other conventional approaches(2).

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Review on: walnut Shell

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Abstract: Walnut (Juglansregia L.) is a very popular and widely consumed crop, not only as dry fruit but in form of green walnuts, shells, kernels, barks, green walnut husks (epicarp) and leaves have been used in both cosmetic and pharmaceutical industries and also in agricultural industries & fuel industry, but there is no major emphasis is done for therapeutic uses.

walnut shell is an agricultural waste having cellulose structure havingrich in total phenolic content responsible for effective scavenging of free radicals . examples in walnut shell: pyroligneous acid ,chlorogenic acid, caffeic acid, ferulic acid, gallic acid, ellagic acid, etc. because of this constituent advancement is required to explore therapeutic uses.

pyroligneous acid is a crude reddish brown liquid produced from dry distillation of biomass during pyrolysis process and this acid is widely used in medicine, food & agricultural. In agricultural it is used to promote rooting and seed germination. in rubber industry it is used as coagulator and anti-fungal agents. Pyroligneous acid is responsible for various biological activities such as anti- microbial and anti- oxidant. For phytochemical screeing and estimation of phytoconstituents analytical methods are used like HPTLC, HPLC ,etc.

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Camphor: A Review on Scientific Evidences and Medical Significance

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Abstract: Camphor (Cinnamomumcamphora) which is obtained from the wood of camphor tree, has been used for centuries and throughout the world as a remedy for treating variety of symptoms such as inflammation, ingestion, infection, congestion, pain, irritation, etc[1].Camphor is readily absorbed from all the sites ofadministration, after inhalation, ingestion or dermal exposure and acts as slight local anesthetic, antimicrobial substance, cough suppressant and suppressor of sexual behaviors and sex hormones. The presence of anti-itch gels and cooling gels with camphor as the active ingredient which produces a feeling of cooling similar to that of menthol[2, 3].The leaf of *Cinnamomumcamphora* contains camphor, as the main component along with cineol, linalool, eugenol, limonene, safrole, α-pinene, β-pinene, β-myrecene, α-humulene, p-cymene, nerolidol and many more[4]. The present review emphasizes on compilation of different chromatographic method developed in order to estimate content of camphor[5]. The compilation also focuses on common interest of common people and scientists to explore the use of camphor for daily minor problems as well as treatment of life threatening disease. More attention is are required to develop the standardization parameters and separation of phytoconstituents using various hyphenated techniques.

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Medicinal chemistryapproaches of PI3K inhibitors as anti-cancer agents.

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Abstract: One of the most commonly triggered pathogenic signalling cascades in human malignancies is the phosphatidylinositol-3 kinase (PI3K) pathway.Thephosphoinositide 3-kinases (PI3Ks) are a large family of lipid enzymes that phosphorylate on the plasma membrane the 3 '-OH class of phosphatidylinositols.PI3K is mutated in extensive variation of cancers including breast, prostate ovarian etc. Over the years, studies are still underway to find more efficient and selective PI3 K inhibitors or dual PI3 K inhibitors to overcome current inhibitors resistance.At the forefront of educational and industrial medicinal chemistry the search for novel PI3K inhibitorsare rapidly expanding due to the significant role of PI3Ks as intracellular signal transducer enzymes. In the present compilation, we are focusing on the three main classes of PI3K inhibitors showing active antitumor activity.Furthermore, SAR of the classes, and design of new isoform-selective inhibitors in medicinal chemistry will be discussed.

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Antibody Drug Conjugate for Cancer Therapy

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Abstract: The chemotherapeutic drug are effective in cancer treatment but they cause side effects in a wide range. The antibody drug conjugates(ADC) are new class of immunotherapeutic drug which are conjugates of monoclonal antibody to cytotoxic drug using linkermolecule. The monoclonal antibody of ADC are effective in binding to highly expressed receptor on cancer cell andget internalized into the tumour cell to release the cytotoxic drug. The advancement in biotechnology and bioengineering had led the evolution of specific attachment of ADC to the target site and increase the stability of linker molecule which prevents the premature detachment of cytotoxic payloadsto linker molecule and prevent unwanted systemic side effects.Hence for the development of ADC require a proper selection of monoclonal antibody, a suitable linker and a proper drug to antibody ratio should be maintained.Recently a large number of ADC are under clinical trials ,there are two ADC drug which have got FDA approval they arebrentuximabvedotinuse in hematologic malignancies and ado-trastuzumab emtansine for solid tumour are now in clinical use. In this poster review the mechanism of action, type of linker molecule and monoclonal body employed.

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Application of current nanotechnology-based approaches in treatment of colorectal cancer (CRC)

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Abstract: Recent statistics have reported colorectal cancer (CRC) as the second leading cause of cancer-associated deaths in the world. Alike other forms of cancers, diagnosis at the early stages of CRC may help to reduce the mortality and associated complications. However, the conventional diagnostic tools and techniques often lead to misdiagnosis, fail to differentiate benign from malignant tissue or diagnose only at an advanced stage of the disease. From the treatment perspective, surgical intervention is obligatory in some cases. However, for the treatment of irresectable CRCs and as an adjuvant therapy to surgery, other forms of therapies including chemotherapy, immunotherapy, and radiotherapy have been employed. Although being beneficial for most of the patients in terms of prognosis, the quality of living of the CRC patients is highly compromised owing to toxicity issues and relapse.

Employing nanotechnology-based approaches has demonstrated promising outcomes in the prevention, diagnosis, and treatment of many forms of cancer including CRC. Nanotechnology-based diagnostics and therapeutics can surmount major drawbacks of traditional therapy as well as help in the prevention of CRC. Nanocarriers render advantage of early diagnosis, increased targetability to the tumor sites, improved drug bioavailability, controlled and prolonged drug release and reduced adverse effects. This paper emphasizes on molecular mechanisms involved in the pathogenesis, conventional approaches and issues confronted thereby. It provides an outlook on the application of current nanotechnology-based approaches for prevention, early diagnosis, and treatment and future perspectives of this outrageous disease.

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Role of Liver X Receptors in Cardiovascular Diseases

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Abstract: Cardiovascular diseases (CVDs) are leading cause of death around the globe with an estimated rate of around 17.9 million deaths, of which 85% mortality rate is due to heart attack and stroke. Currently used antihypertensive, antilipidemic, antiplatelets and antithrombotic agents have certain side effects such as irregular heartbeats, dry mouth, cough, rhabdomyolysis, sexual dysfunction, etc. various heart surgery can cause certain damages to tissues and may lead to death. Nuclear receptors like liver X receptors (LXRs) has been studied recently in metabolic disease, Alzheimer's disease, inflammatory disease and anti-inflammatory disease. LXRs also called as "cholesterol sensor" as found play significant role in maintaining lipid homeostasis and also regulate carbohydrate metabolism. Cholesterol derivatives, oxysterols were the first endogenous ligand found to activate LXRs whereas T0901317 and GW3965 were the potential synthetic LXR agonist reported. Beside these, there is various evidence to suggest that LXR may exert their beneficial role in heart disease. We reviewed recent data that shows a direct role of LXR agonist in heart, cardiomyocyte damage due to myocardial ischemia, diabetic cardiomyopathy, cardiac hypertrophy, fibrosis and angiogenesis. LXRs found to decrease infarct size, increase left ventricular contractile function, decrease high glucose-induced cardiomyocyte injury, and increase GLUT4 expression. Various accumulating evidences support that LXRs may represent a novel potential therapeutic target for various cardiovascular diseases.

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Formulation, Characterization and Optimization of Matrix-Type Transdermal Patches Containing Clozapine using the Box–Behnken experimental design

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Abstract: Schizophrenia is a severe form of mental illness affecting about 21 million people worldwide. It is more common among males (12 million), than females (9 million). The present research work was intended to develop and optimize transdermal matrix patch of clozapine using Box–Behnken experimental design (BBD) for improved bioavailability and patient compliance as compared to oral formulation.The 3-factor, 3-level BBD was employed to investigate the combined influence of formulation variables on flux, tensile Strength and *in vitro* drug release. The generated polynomial equation was validated and desirability function was utilized for optimization. Optimized formulation evaluated for physicochemical characterization, FTIR, DSC, *in vitro* drug release, permeability enhancement potential by ex vivo and stability studies.

The results of the formulation trials showed that as the polymer concentration increases tensile strength increases while flux and % drug release after 20 h (Q_{20}) decreases.Optimized formulation was stable up to six months in accelerated condition. Observed and the predicted values of the responses were found to be in good agreement. Results indicated that the transdermal application of clozapine can be promising route of administration for improved bioavailability by escaping first pass metabolism and hence for better management of schizophrenia in long-term basis along with improved patient compliance.

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OLAPARIB NANO-DRUG DELIVERY SYSTEM FOR CANCER THERAPY

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Abstract: In recent time cancer cell have found to bear BRCA1 or BRCA2 mutations on genome have potentially exhibitPARP1 as the only enzyme found to repair DNA in cancer cell. First generation Strategic targeted therapy hadnot been found to be affective towards off target so PARP inhibitor have found it. development among these class of drug,Olaparib has found to be the most successful candidate. Olaparib show regression of the tumor cell and cause it death as it doesn't allow DNA to repair.Oral administrationhad found to be less therapeutic effective as compared to the resultswhich obtain by its nano form. As the nano form shows 10% cell death with irradiation Alone compare to the untreated cell. The effect of irradiation is observed to be the greatest with nano-olaparib (50% Cell death) treated cells compared with olaparib (20% cell death). In this poster review regarding the mechanism of action of Olaparib,it's nano formulation and various therapeutic effects.

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Analytical tools for the characterization of viral vectors

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Abstract: The tools which are commonly used to deliver genetic material into cells by specialized molecular mechanisms to efficiently transform their genomes inside the cells which introduce gene of interest are called viral vectors. Viral vectors have frequently been applied in gene therapy with the final goal of treating various neurological diseases, metabolic disease and cancer. Adenosine associated virus (AAV) based vectors have been used for desired human gene therapy. By the application of AAV vectors promising results have been obtained from phase 1 and phase 2 clinical trials including Leber's congenital amaurosis, Hemophilia. So, appropriate analytical approaches should be developed to achieve safety, potency and purity. Process Analytical Technology (PAT) was introduced by FDA to ensure Critical Quality Attributes (CQAs) that are important for monitoring of viral vectors during manufacturing which includes Viral Potency, Identity, Quantity, Process residuals, aggregation, empty capsids, protein content and product safety. Analytical Methods used for Viral Vector Characterization are:

Quality	Analytical Method
Identification of viral vectors	Mass Spectroscopy, Western blot, Genome Sequencing (Next-Generation Sequencing), Real time PCR, Optical density.
Potency	Plaque Forming Assay, Fluorescence foci assay, Transmission electron microscopy for process related impurity
Purity	qPCR, ELISA, For Sterility (LAL Test and Rabbit Pyrogen Assay)
Safety	Southern Blotting, Potentiometry, Osmolality
Stability	Light Microscopy, AUC (Analytical Ultracenrifugation)

Keywords: Viral Vectors, AAV, Process Analytical Technology (PAT), human gene therapy.

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EVALUATION OF ANTIOXIDANT EFFECT OF FERULIC AND FOLIC ACID ON ALCOHOL INDUCED LIVER INJURY IN WISTAR RATS

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Abstract: Objective: The present study aimed to investigate hepatoprotective and antioxidative effects of Ferulic acid (FLA) and Folic acid (FA) against oxidative stress in Wistar rats with alcohol induced liver injury and underlying mechanisms.

Materials and method: Female Wistar were treated with Ferulic acid (20 mg/kg, p.o.) and Folic acid (1 mg/kg, p.o.) and standard (400 mg/kg) for 6 weeks evaluated against alcohol induced (5 g/kg, p.o.) groups. Rats were divided into six groups Normal control, Alcohol treated (5g/kg), Standard, Ferulic acid, Folic acid, Ferulic + Folic acid. The hepatoprotective evaluation was estimated by biochemical parameters: SGPT, SGOT, albumin, total protein, Bilirubin and C - reactive protein. Furthermore oxidative stress, hematological and histopathological parameters using hematoxylin, eosin, Masson's trichome staining and Congo-red staining was performed.

Result: Alcohol induced liver injury significantly increased SGOT, SGPT, bilirubin and C - reactive protein and decreased total protein and albumin levels. On treatment with Ferulic acid and Folic acid revealed significant reduction in serum SGPT, SGOT and total bilirubin with increase in total protein and albumin levels to normal treated groups. Hematological results showed decrease in significant RBC indices, differential WBC count and platelet counts. Histopathological observations showed prevention of liver against damage.

Conclusion: It is concluded that liver function was preserved by determining morphological and structural view. The decrease in oxidative stress may be due antioxidative activity. The histopathological and biochemical parameters' results showed significant improvement after treatment with Folic and Ferulic acid and their combination at the dose 1mg/kg and 20 mg/kg.

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Drug discovery & development targeting G-Protein Coupled Receptor 40 (GPR 40) for Type-2 diabetes mellitus (T2DM)

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Abstract: Diabetes is a chronic disease that occurs either when the pancreas does not produce enough insulin or when the body cannot effectively use the insulin it produces. Insulin is a hormone that regulates blood sugar. There are two types of diabetes type 1 (known as insulin-dependent, juvenile or childhood-onset) is characterized by deficient insulin production and type 2 (formerly called non-insulin dependent, or adult-onset) results from the body's ineffective use of insulin. According to WHO, in 2016, an estimated 1.6 million deaths were directly caused by diabetes, another 2.2 million deaths were attributable to high blood glucose in 2012.Free fatty acid receptor 1, also known as GPR40, is a class A G-protein coupled receptor that in humans is encoded by the FFAR1 gene. It is strongly expressed in the cells of the pancreas and to a lesser extent in the brain. Fatty acids can acutely stimulate insulin secretion when glucose is present with long-chain SFA, MUFA, or PUFA. There are many researches on going on this receptor. First drug is TAK-875, which was withdrawn from phase 2 due to hepatotoxicity and many others are withdrawn for the same reason. Herein, we describe the various drugs under pipeline as well as enlist drugs under development with their efficacy in treating T2DM.

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ROLE OF NIMA RELATED KINASE 2 (NEK-2) IN LUNG CANCER

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Abstract: Lung cancer is the lethal of all cancers in the world (International Agency for Research on Cancer (IARC), 2018). Previous studies have also found that NEK2 protein expression is elevated 2-5 fold in cell lines derived from a variety of human tumors, including those of the ovary, breast and prostate. The present study showed that NEK2 expression was significantly upregulated in NSCLC (Zhong, Guan, Liu, & Zhang, 2014). Nima related kinase 2 (NEK2) is a serine / threonine protein kinase and it is associated with the family of nima related kinase (Nek). The main role of Nek2 in regulation of cell cycle. NIM suggest “never in mitosis”. It anchoring cell cycle progression from G2 to M phase. The role of Nek2 in cell cycle such as centrosome separation and duplication, spindle assembly checkpoint, kinetochore microtubule attachment, and microtubule stabilization (Meng et). Overexpression of Nek2 is also found in lung cancer. High Nek2 levels produce chromosomal instability (CIN) and aneuploidy, which will finally responsible for tumorigenes.Once the NEK2 overexpressed it activates various molecularsignaling pathways viz. KRAS, PI3K/AKT/mTOR, Wnt, and EGFR (Das et al., 2013).The current treatment and therapies of lung cancer include thoracic surgery, radical radiotherapy, radiofrequency / microwave ablation, systemic therapies. In lung cancer first line and second line therapy is also available (Soulier & Moro-Sibilot, 2009). Personalized medicines is a new trend for treating lung cancer patient in which NEK2 overexpressed.

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Nanocarriers involved in Transdermal drug Delivery

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Abstract: Transdermal drug delivery represents an extremely attractive and innovative route across the skin owing to the possibility for achieving systemic effect of drugs(1).Transdermal drug delivery systems have been around for decades, where current technologies objective is toenhance skin penetration of larger, hydrophilic drugs and macromoleculesfor disease treatment and vaccination(2).Transdermal drug delivery would be on focal as it provides patient compliance, first-pass metabolismavoidance, local targeting and reduction in toxic effect related to various categories of drugs like, anti-inflammatory,antimicrobial, anaesthetic, anticancer *etc*(1).But the main advantages of TDDS is that it lie under category of controlled drug delivery, inwhich the aims to deliver the drug through the skin in a predetermined and controlled rate(3). As to increase the range of drugs available for transdermal delivery, the use of nanocarriers has emerged as an interesting and valuable alternative for delivering lipophilic and hydrophilic drugs throughout the stratum corneum , as these nanocarriers : nanoparticles,dendrimers, liposomes, etc can be made of a variety materials, and they are very different in structure and chemical nature(4)(5). They are too small to be detected by the immune system, and furthermore they can deliver the drug in the target organ using lower drug doses in order to reduce side effects(5).So as per multipleresearch one can conclude that confirm the wide application of nanocarriers for transdermal deliveryof drug(1).

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MEDICINAL CHEMISTRY APPROACHES OF SURVIVIN INHIBITORS

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ABSTRACT: Survivin is the smallest member of inhibitors of apoptosis protein family. It is also referred as BIRC5 gene that is baculoviral gene. Survivin is highly expressed in cancerous cells and fetal tissue while it is less detectable in normal cells which is useful for the providing a new target for cancer therapy. It is also helpful for the discrimination of cancerous cells and normal cells. Survivin protein is localized into the mitotic spindle of the microtubule by interaction with tubulin. The role of Survivin is to regulate the cell cycle particularly at G2 phase, inhibition of apoptosis and regulation of metastasis. The various actions of Survivin can be inhibited by various types of inhibitors such as YM155 (Currently in Phase II). It is one of the type of inhibitor that reverses Rapamycin resistant renal cell carcinoma. Other inhibitors which are under clinical trials are Flavopiridol (Phase-II), Terameprocol (Phase-I), MK-2206 (Phase-II) etc. In this review we will discuss the role of survivin in cell division, inhibition of extrinsic and intrinsic apoptosis pathway as well as the mechanism and chemistry of Survivin inhibitors on different cancerous pathways.

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EFFECT OF TOLUENE, AN ENVIRONMENTAL TOXIN IN CNS FUNCTIONS

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Abstract: In this study the acute toxicity of toluene on the brain has been investigated using rats via histopathological, bio-chemical and neurobehavioral tests. The Intracerebroventricular route (ICV) was utilized for induction of the neurotoxin directly into the brain. Levels of various important neurotransmitters such as dopamine (DA), Acetylcholine (Ach) and Serotonin (5-HT) were ascertained in order to ascertain the extent of the biochemical damage. Amount of dopamine, secreted from the substantia nigra and acetylcholine levels were detected to be significantly lower in the toluene-administration group than in the control group. Severe degeneration in the structure of brain cells and also dispersed cell borders were observed. Furthermore, abnormal malformations of the nuclei structure of the oligodendrocyte cells were observed. Bodies of the sequential neurons of the hippocampus in the toluene-administration group were distinctly structurally damaged compared to the control group. In addition, cytoplasm of the cortex cell showed nuclear atypia and necrosis in the experimental group. These results indicate changes in OS parameters with toluene exposure resulted in oxidative damage in the entorhinal cortex of experimental group rats. These changes in OS parameters and neurotransmitter levels are possibly related to neurobehavioral and neurophysiological effects of toluene in the animal model.

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Treatment of atomic dermatitis by Nanostructured LipidicCarriers (NLC)

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Abstract: Atopic dermatitis is very common skin disorders that occurs mostly in developed countries. It will affect up to 20% of children and 1 to 2% of adults. Mostly hand dermatitis is widely spread and has high chances of relapses clinical course. Current therapies to treat topical dermatitis includes corticosteroids, that is first line therapy; in addition to this calcineurin inhibitors (TCIs), first generation antihistaminic and phototherapy. In spite of this, Atopic dermatitis may cause some undesirable and potential side effect. Now-a-days nanotechnology-based dosage forms are being explored to treat symptoms of Atopic dermatitis with better efficiency. These will also improve the topical and systemic penetration of drug particles. Specifically, lipid based nano carrier system (Nanostructured lipid carrier - NLC) provides promising result in drug penetration and drug resident time at inflamed tissue also increased due to lipidic carrier system. A new generation Nano lipid carrier (NLC) has special lipidic structure into this drug will incorporated so drug loading capacity will also increase. This system contains low viscosity aqueous dispersion, which is usually available as semi solid formulation with proper consistency that can easily apply to the skin.

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P-141

AI ADVANCES BEYOND DRUG DISCOVERY

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Abstract: ARTIFICIAIINTELLIGENCE has recently been developed into a sizzling topic in the area of medical care industry and becoming prime drivers of efficiency for forward-thinking pharma companies. Having proven how AI can be leveraged to make data-driven decisions faster and ramp up R&D, drug developers are now discovering a limitless range of novel and beneficiaI uses.
AI Expanded in terms of exponential growth in high performance computing, data communication, clod technology and big data storage. And that brought AI into limelight since then the AI is expanding for drug discovery are rising.

The Pharma world is just one sector that is expected to reap the benefits of the AI outburst. The biopharmaceutical industries are making efforts to approach AI to enhance drug discovery process, reduce research and development expenses, diminish failure rate in clinicaI trials and ultimately generate superior medicines.

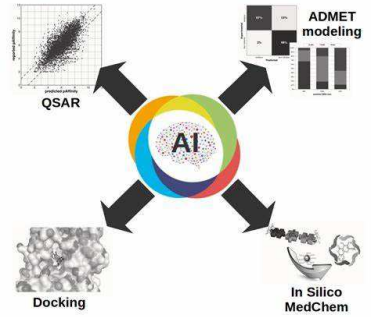
AI based startup companies makes more eye rolling over **DRUG**

DISCOVERY. in the workplace, thanks to **OPTICAL CHARACTER RECOGNITION (0CR)** applications and other enhanced data-capture tools.

AI i AI is enabling professionals in pharmaceutical occupations to be people again s not just eliminating staffer's monotonous tasks — it's aIso helping them locate data patterns faster, interpret data analyses sooner, and make more informed and timely decisions.

"(walker Osborn explain that AI can be used for target identification, insilicomedicine of Baltimoredrug design and development, big data analytical, prediction of study risks, patient matching and more……)"
Other developing AI applications around the pharma world include:

Diagnostic machines, drug delivery machines, Genetic research applications, automated machines which give detail about drug-drug interaction food-drug interaction to direct patient for better output.



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REGULATORY PATHWAY FOR BIOTECHNOLOGY PRODUCTS IN INDIA

TASNEEM RANGWALA

REGULATORY AFFAIRS SEM-3

Abstract: Biotechnology, in India was observed solely in 1997 by coming in market indigenously developed recombinant DNA technology-based product, the hepatitis B vaccine, by Shantha Biotechnics. the Genetic Engineering Approvals Committee, a body under the Ministry of Environment and Forests look after the approval of genetically engineered products in India. Now is the time they have taken concrete steps for more detailed regulatory system for growing of biotech industry. Modern biotechnology includes Genomics, proteomics and bioinformatics. The Indian market provides opportunities to produce and sell vaccines and therapeutics that respond to the needs of the millions of poor in India. DBT is main regulator for biotech products in India. Development for the products are reviewed by Recombinant DNA Advisory board (RDAB) at both national and international levels. In ongoing projects safety aspects are regulated by RCGM (review committee on genetic manipulation) and other committees given.

Keywords: Biotechnology, approval, review process, development

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Eugenol improves motor defect and blood brain barrier disruption induced by traumatic brain injury.

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Abstract: Background: Traumatic brain injury (TBI) occurs on transmission of the external force to the head which can lead to cognitive disabilities either short term or long term. TBI was induced by using the weight drop method. Blood brain barrier disruption in the secondary injury stage which starts after several week of injury is very crucial to maintain therapeutically. This disruption of blood–brain barrier (BBB) causes subsequent edema, leukocyte recruitment to the injury site, and induction of proinflammatory and potentially neurotoxin mediators. We here investigated the role of eugenol in inhibiting blood brain barrier disruption and improving motor defect in rat.

Method: Twenty Four adult Sprague-Dawley rats of either sex (250-400 gm) were divided into three groups. Traumatic brain injury was induced by using weight drop method. Weight of 350gm was impacted on the rat's brain; also rat's forebrain was covered by a metal helmet. Group 1 is control group with n=8 no induction or treatment was given. Group 2 is the TBI group, Group 3 is the treatment group where pre- treated rat with eugenol undergoes weight drop method for trauma induction. Behavioural analysis was done on pre and post trauma induction. Blood brain barrier integrity was analysed by estimating brain water content and estimating blood brain barrier integrity study.

Results: Traumatic brain injury by weight drop method on rat causes increase in the blood brain barrier permeability, brain water content (edema) and impaired cognitive function as per results. Administration of eugenol before weight drop method proves to be significantly improving the motor function and BBB integrity.

Conclusion: Traumatic rat when pre-treated with eugenol improves the motor defects and BBB disruption & integrity.

Keywords: Traumatic brain injury, Weight drop method, Eugenol, Blood brain barrier.

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Design and Synthesis of Nitrogen-containing Heterocyclic for the Inhibition of Telomerase in the treatment of Cancer

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Abstract: Telomerase, a widely expressed hallmark responsible for replicative immortality in 80-90% of malignant tumors.[1] Cancer cells produce telomerase, which prevents telomere shortening by adding telomeres sequences beyond the Hayflick's limit; that enables them to divide uncontrollably. Nowadays, distinctive features of telomere and telomerase preferred as the target for the development of novel chemotherapeutic agents.[2] In this work, Pharmacophore, 3D-QSAR, molecular docking as well as *in-silico* ADMET studies were performed for the designing of novel potent compounds. Nine telomerase inhibitors reported in the clinical trials and non-clinical stage in various literature, were selected for the generation of a pharmacophore model. Phenylacetamide was identified as a pharmacophore unit responsible for the inhibition of telomerase. In 3D-QSAR, 37 quindoline, quinolone, and acridine derivatives reported as telomerase inhibitors in diverse literature were selected for the ligand-based 3D-QSAR study. Statically significant CoMSIA with a q2 value of 0.662 and higher predictability with r^2_{pred} value of 0.560 participated in the generation of contour maps that reveal the information about the favourable substitution over the heterocyclic moiety for the enhancement of telomerase inhibition effect. Combination of Novel pharmacophore moiety with favourable anti-telomerase substitution help to design the new molecules. The biological interaction of design molecules with telomerase were estimated by docking of that molecule with target PDB (3DU6 and 5CQG). Effect of design molecules over the biological system were determined by Osiris property explorer. Performed the synthesis of those design molecules that shows maximum biological interaction with minimum toxicity in wet lab synthesis.

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Role of Liver X Receptors in Cardiovascular Diseases

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Abstract: Cardiovascular diseases (CVDs) are leading cause of death around the globe with an estimated rate of around 17.9 million deaths, of which 85% mortality rate is due to heart attack and stroke. Currently used antihypertensive, antilipidemic, antiplatelets and antithrombotic agents have certain side effects such as irregular heartbeats, dry mouth, cough, rhabdomyolysis, sexual dysfunction, etc. various heart surgery can cause certain damages to tissues and may lead to death. Nuclear receptors like liver X receptors (LXRs) has been studied recently in metabolic disease, Alzheimer's disease, inflammatory disease and anti-inflammatory disease. LXRs also called as "cholesterol sensor" as found play significant role in maintaining lipid homeostasis and also regulate carbohydrate metabolism. Cholesterol derivatives, oxysterols were the first endogenous ligand found to activate LXRs whereas T0901317 and GW3965 were the potential synthetic LXR agonist reported. Beside these, there is various evidence to suggest that LXR may exert their beneficial role in heart disease. We reviewed recent data that shows a direct role of LXR agonist in heart, cardiomyocyte damage due to myocardial ischemia, diabetic cardiomyopathy, cardiac hypertrophy, fibrosis and angiogenesis. LXRs found to decrease infarct size, increase left ventricular contractile function, decrease high glucose-induced cardiomyocyte injury, and increase GLUT4 expression. Various accumulating evidences support that LXRs may represent a novel potential therapeutic target for various cardiovascular diseases.

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DNA NANOTECHNOLOGY: A STEP TOWARDS THERANOSTIC PLATFORM FOR VARIOUS DISEASES

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ABSTRACT: DNA nanotechnology is the design and manufacture of artificial nucleic acid structures for technological uses. In this field, nucleic acids are used as non-biological engineering materials for nanotechnology rather than as the carriers of genetic information in living cells(Loizidou & Seifalian, 2010)[2].DNA nanostructures are nanoscale structures made of DNA, which acts both as a structural and functional element. Nitrogenous bases are notable molecular tools for designing functional supramolecular assemblies. Some of the basic and emerging assembly principles for construction of DNA nanostructures are hybridization, base stacking/shape complementarity, and protein-mediated(Hu & Niemeyer, 2019)[1]. The advancement in nano technology helps in the treatment of neurodegenerative disorders such as Parkinson's disease and Alzheimer's disease. DNA nanostructures are also used in treatment of tuberculosis and various cancers. The advantage of nanotechnology is that they facilitate the passage of drugs through the blood brain barrier (BBB), enabling targeting before body degradation, and increasing therapeutic efficacy, compared to conventional pharmaceutical dosage forms(Seeman, 2003)[4]. It offers simple yet powerful design techniques for self-assembly of nanostructures with unique advantages and high potential in enhancing drug targeting and reducing drug toxicity. DNA nanostructures with precisely engineered, controllable size, shape, surface chemistry, and function are being used. Potent anticancer drug molecules, including Doxorubicin and CpG oligonucleotides, have been successfully loaded on DNA nanostructures to increase their cell uptake efficiency. These advances have implicated the bright future of DNA nanotechnology- enabled nanomedicine(Mathur & Medintz, 2019)[3](Upadhyay, 2014)[5].

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REVIEW ON BIOSIMILAR REGULATIONS AND APRROVAL OF CYTOKINES AND PEGYLATED CYTOKINES IN INDIA, US, JAPAN AND EUROPE

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ABSTRACT Biosimilars are biologic medical products whose active drug substance are made by a living organism or derived from a living organism by recombinant DNA or controlled gene expression methods. A biosimilar is a biological medicine that is similar, but not identical, to an already registered reference biotherapeutic product in terms of quality, safety, and efficacy. Cytokines are the large group of proteins, peptides or glycoprpteins such as interlukins and interferons that are secreted by specific cells of immune system. Cytokines are smaller in size compare to proteins and monclonal antibodies. The number of biosimilars products approved in US are 25; in India are 70; in Europe are 19 and in Japan are 7. Some of the examples of the drugs that are approved in market are: Glaritus, Intacept (India); Ziextenzo, Eticovo (US); Benepalietc, Erelzi (Europe); Agalsidase Beta BS [JCR], Etanercept [YLB113] (Japan), etc. Biologics are different from biosimilars as biologics are very large and have complex molecular structures. There are different regulatory bodies and regulations for the biosimilar approval in different countries. The approval of biosimilars is needed to bring safe, cost-effective and effective biosimilars in the market.

KEY WORDS: Biosimilars, Biologics, Regulations, Cytokines, Pegylated Cytokines.

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New emerging target in cancer immunotherapy: TIM3

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ABSTRACT: In recent years, immune checkpoint inhibitors, such as programmed death receptor 1 (PD-1) and programmed death-ligand 1 (PD-L1), has shown promising therapeutic resultsand revolutionized the treatment of many cancer types.Patients treated with anti-PD-1 or anti-PD-L1 monoclonal antibodies will face the resistance problems. It is reported that TIM-3 expression was amplified when patients expressed with the antiPD-1 adaptive resistance.TIM-3 could be animportant target in cancer because of its expression on a various T cell. TIM-3 was also expressed on myeloid cells, such as DCs, macrophages, and monocytes.In antitumor immune responsesmediated by innate immune cell,TIM-3 has a significant role.Recent studies have emphasized that TIM-3 has avital role to play in exhaustion of T-cell and correlates with the consequence of anti-PD-1 therapy. TIM-3 targeting might be a significant approach for cancer immunotherapy. A brief discussion of one of the most promising immune-checkpoint targets currently under investigation, the T-cell immunoglobulin and mucin domain-3is stated in this presentation.

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Tyrosine kinase inhibitor in combination with PPAR-γ agonist: Directing metabolic dysfunction through AMPK pathway

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ABSTRACT: Thiazolidinediones exhibits potential improvement in glycemic control and insulin sensitivity by binding withPPAR-γ receptors. Molecular docking studies suggest that tyrosine kinase inhibitors interact with PPAR-γ in ligand binding domain with high predictive values.We studied the effect of Tyrosine Kinase Inhibitor and combination on diabetes in db/db mice. Dasatinib was administered at the dose of 2.5mg/kg p.o., gallic acid 100mg/kg p.o. and pioglitazone 20mg/kg p.o. and their combinations into db/db mice for 4 weeks. At the end of treatment effect on glucose homeostasis was measured using glucose tolerance test and assessment of insulin sensitivity test. The liver inflammation and lipid infiltration in adipocytes were assessed by histopathology using H & E staining.The combination of dasatinib with gallic acid and pioglitazone produced statistically significant improvement in blood glucose levels after 4 weeks of treatment as compared to dasatinib alone. Combinations have also shown decrease in body weight. Akt phosphorylation after insulin administration was improved by both combination therapies. Lipid infiltration and inflammation of liver cells were decreased by both combination therapies which was shown by decreased adipocytes size and hypertrophy of liver cells.Combination of tyrosine kinase inhibitor and PPAR-γ agonists ameliorated insulin resistance by activating phosphorylated form of AMPK, Akt and increased expression of Ki76 in db/db mice. Thus combination of tyrosine kinase inhibitor and PPAR-γ could be used as therapeutic agents against type 2 diabetes and metabolic syndrome.

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Pharmacodynamic and Pharmacokinetic study of novel nanoparticles of Irinotecan Hydrochloride in fibrosarcoma

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ABSTRACT: Irinotecan is a highly effective anti-cancer agent but reported to have poor bioavailability, large dose is require obtaining good therapeutic effect. Therefore, aim of present study is to develop drug entrapped gelatin nanoparticulate system for targeted drug delivery to specific site of action, improve drug stability, retention time and with no or less side effect. Nanoparticle of irinotecan hydrochloride is formulated by nanoprecipitation method with gelatin as a biodegradable polymer and folic acid as targeting molecule. The drug characterization and *In vitro* drug release study was carried out. For *in vivo* evaluation of nano-formulation, fibrosarcoma was induced by injecting WEHI 164 cell line via sub-cutaneous route. After 8 to 10 days of tumour incidence treatment was started by i.v. route for three times in three weeks. Daily tumor size and body weight was measured. After completion of treatment period all the animal were sacrificed and samples were collected and stored for further studies. Pharmacokinetic and bio-distribution of novel nanoparticles was conducted. Drug loading efficiency of G-FOL-IRI was significantly higher than G-IRI. In vitro drug release showed that formulation follows controlled release kinetics. *In vivo* efficacy study IRI, G-IRI and G-FOL-IRI possess inhibitory effect on tumor volume. Among them folate grafted gelatin NP showed statistically ($p<0.05$) significant decrease in tumor volume as compared to other groups. Pharmacokinetic and biodistribution study showed that G-FOL-IRI has highest plasma half-life and retention time as compared to IRI, G-IRI. These results suggested that folate targeted nanoparticle could be useful for targeted delivery system for treatment of fibrosarcoma.

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Neuroprotective Effect of *Butea Monosperma* in Sporadic Alzheimer's Disease

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ABSTRACT: Background: Sporadic Alzheimer's disease, an age-associated dementia and neuronal loss characterized by cognitive impairment. Epidemiology suggests that around 4.1 million Indians suffer from Alzheimer's associated dementia. Currently available treatment prevents worsening of condition with many side effects. *Butea monosperma commonly known* palash belonging to *leguminosae* family has been accepted traditionally in form of natural medicine and flowers are used for *Antifungal activity, Anti-inflammatory activity, Neuroprotective activity* etc. Objective of study was to evaluate Neuroprotective effect of BTM in Streptozotocin induced SAD.

Materials and methods: SAD was induced by icv administration of STZ (3 mg/kg). Animals were divided in Group 1 normal control, Group 2 sham control, group 3 disease control, group-4 disease control with standard treatment donepezil at dose 10 mg/kg. Group 5 (DC+ BM100), group 6 (DC+BM200) and group 7 (DC+BM400). Behavioral tests were done, animals were sacrificed, and biochemical and histopathological evaluations were done.

Results: Percent alteration score and **Total arm entry** in Y maze was reduced in DC group compared to NC group while it was increased in treatment groups compared to DC group.

Escape latency test in water maze, animals observed for improvement in escape latency and after removal of hidden platform, treated animals observed for improvement in probe trial test when compared with DC group which indicates improved spatial recognition memory.

CRP levels, AchE activity significant increased levels in DC group and decreased in treatment groups.

Brain Mitochondrial ATPase assay, a significant increase in levels in treatment groups compared to NC group.

Oxidative stress parameters, MDA levels were found to be lowered and SOD, GSH, and catalase levels were significantly increased in treatment groups.

Histopathological study, change in hippocampus with damaged cells increased in disease group and less damage in normal and treated group.

Conclusion:

Study suggests that BTM showed protective effect against STZ induced AD that in turn reflects improvement in spatial and working memory through strong neuronal connectivity.

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CALIXARENE – A BLOCKBUSTER ENTITY IN PHARMACEUTICAL SCIENCES

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Abstract: Persistent research and development in fields like science and technology have revolutionized the globe in the way things are perceived and addressed. The notion of a fast lifestyle and urge to get things done "quickly" has hence increased. This quick lifestyle has eventually led to the occurrence of health issues rather earlier than usual. It is evident that a healthy state of the body is pivotal for efficient activity and productivity. It thereby, necessitates the evolution of medical sciences in the way such disorders are treated as well.One such approach is by enhancing the rate of curing action of medicinal drugs. It could be done by sending more drug molecules per dose to the target organ thereby, increasing the drug action and elevate the process. This can be achieved by a polymeric ligand - Calixarenes.Calixarenes are like a molecular "bus" that can bind with multiple drug moieties simultaneously and transport them to their respective site of action. This blockbuster entity can possibly be an apt solution to address the issue of rapidly treating numerous diseases. This basket, consisting of cyclic oligomers, takes up the shape of a vase that plays a significant role in shaping the entire architecture for its function in host-guest chemistry.So far, it has been found that calixarenes possess an appreciable anti-bacterial activity, with an additional ability to mimic a few superior antibiotics as well. Moreover, calixarenes have also shown their ability to treat disorders like tuberculosis, fungal infections, inflammatory disorders and many more. In the case of anti HIV, it is possible that nucleotide-calixarene conjugates could open a new dimension of antiviral treatment.

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Superparamagnetic Iron Oxide Nanoparticles Induced Hyperthermia: A novel Approach for Extirpation of Tumour in Head & Neck Cancer

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Abstract: Head and neck cancer is a broad term that encompasses epithelial malignancies that arise in the paranasal sinuses, nasal cavity, oral cavity, pharynx, and larynx. These epithelial malignancies are Squamous Cell Carcinoma of the Head and Neck(SCCHN) , important factors aretobacco and alcohol consumption and few evidences has documented human papillomavirus (HPV) as a cause of SCCHN(Argiris, Karamouzis, Raben, & Ferris, 2008)[1].Superparamagnetic Iron Oxide Nanoparticles(SPIONS) for cancer therapy and diagnosis developed on the basis of their unique physico-chemical properties. A high-frequency magnetic field, SPIONSgenerate heat through oscillation of their magnetic moment. It is a promising method for thermal destruction of tumour cells (Mikhaylov & Vasiljeva, 2011)[7]. Methods used for preparation of SPIONSare: Co-Precipitation, Thermal decomposition, Microemulsion, Sol-gel, etc. The co-precipitation technique, which is the most simple and efficient synthesis procedures, is based on simultaneous precipitation of Fe2+ and Fe3+ aqueous salt solutions via the addition of a weak or strong base. Advantage of co-precipitation technique is that it is cost-effective and high-yield synthesis is possible. Further coating with suitable polymers likePoly(dl-lactic acid),PEG,Dextran, Chitosan,etc. can render the nanoparticles withbetter stability between the particles via steric repulsion, and reduce undesired interactions with plasma proteins and their subsequent opsonisation (Stillfried, Knüchel, Kiessling, & Lammers, 2019)[8](Laurent, Bridot, Elst, & Muller, n.d.)[5](Journal, Khiabani, Farshbaf, & Akbarzadeh, 2017)[4]. The main advantage of SPIONS is that the hyperthermia produced by SPIONS can act as radiosensitizer to radioresistant cancer cells. Tumour cellsare sensitive to hyperthermia but resistant to ionizing radiation which depends on the formation of toxic oxygen radical in well perfused areas(Janko, Ratschker, Nguyen, & Zschiesche, 2019)[3]. Using SPIONS as nanoparticle platform additionally enables monitoring of tumour targeting in magnet resonance imaging resulting in theranostic applications(Wahajuddin, 2012)[9].Disadvantages of SPIONS are Blood vessels and organs deep within the body cannot be targeted by external magnets because of the lack of an effective magnetic field gradient(Laurent, Saei, Behzadi, & Panahifar, 2014)[6]. Another limitation in SPIONS delivery is burst release of drugs grafted onto the SPION surface(Wahajuddin, 2012)[9]. Future perspectives for SPIONS drug delivery is need of monitoring of the burst release effect of SPIONs. Use of crosslinking polymers has demonstrated promising results in controlling the drug release rate(Chen & Chen, 2015)[2](Wu, Wu, Yu, Jiang, & Kim, 2015)[10].

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Blood vessels and organs deep within the body cannot be targeted by external magnets because of the lack of an effective magnetic field gradient

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Atomic Layer Deposition Technique: Novel Coating Technique for Nano Pharmaceutical Coating

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Abstract: Coating is a common pharmaceutical technique of applying a thin polymer-based film to a surface containing active pharmaceutical ingredients (APIs). Solid dosage forms are coated for a number of reasons, the most important of which is controlling the release profiles.(1)The advantages of coating are taste masking, odour masking, physical and chemical protection, protects the drug from the various physio chemical propertiesetc. There are various techniques for tablet coating such as sugar coating, film coating, and enteric coating.(2)But this technique not very much suitable for micro and nano particles for e.g., coating of nanoshells. Recent trends in pharmaceutical technologies are the development of coating methods which overcomes the various disadvantages earlier coating techniques.(1)Atomic layer deposition has been widely used in the electronics industry for decades and is thus well established for larger scale production and automation, while in pharmaceuticals atomic layer deposition is very novel concept.(3) atomic layer deposition is a surface-controlled method of self-limiting layer bylayer coating process.(4) which produces high-quality, ultrathin, and conformal slenderfilms, even on high aspect-ratio structures.(5) It is applicable in nanotechnology and microtechnology,where regulating the thickness of the film at the atomic level is necessary forshrinking the structures.(1)Crucial aspects of this method include surface protection,modification,and functionalization.(6)(7) The moisture-shielding component of this coating has beenused for drug particles (micro- and nanosized) in the pharmaceutical industry.

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PHARMACEUTICAL PRODUCT LIFECYCLE MANAGEMENT

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Abstract: This concept provides opportunity for science and risk based approaches for drug development. The concept is valuable in assessment of chemistry, manufacturing and controls changes across the product lifecycle. A harmonized approach regarding technical and regulatory considerations for lifecycle management will benefit patients, industry, and regulatory authorities by promoting innovation and continual improvement in the biopharmaceutical sector, strengthening quality assurance and improving supply of medicinal products. It provides a framework to facilitate the management of post-approval CMC changes in a more predictable and efficient manner. A strategic approach to lifecycle management, enabling cost reduction and improved compliance.Thus, product lifecycle management is a prerequisite for maximizing a product's lifetime value, improving a company's product development processes, using product-related information to make better business decisions, and delivering greater value to customers.

As a concept, Pharmaceutical companies are now determined to extend the life of their drug beyond patent expiration, devising strategies to manage the lifecycle of their most important medicines that begin in the clinical phases. PLM has become a necessity to the continued success of pharmaceutical companies. Companies that have instituted a comprehensive lifecycle management strategy and a detailed plan to guide their progress toward their goal are reaping financial and clinical rewards. Successful PLM involves the continued development of scientific, technical, regulatory and marketing strategies that enhance the value and extend the life of medicines. PLM was evolved in the 1990s and has played an important role for manufacturing companies. During the last two decades, changes have taken place due to modified regulations, technological advancements and globalization in the last decade, PLM was viewed by industry as a tool to extend lifecycle of products while regulators found it a kind of antitrust activity to create monopoly. However, the previous decade has witnessed the transformation in their views.

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1. https://database.ich.org/sites/default/files/Q12_EWG_Annexes.pdf
2. http://www.eurekaselect.com/138430/article?trendmd-shared=3
3. https://www.pharmatutor.org/articles/product-life-cycle-management-in-pharmaceuticals-review

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Medicated Chewing Gum : A Potential Drug Delivery System

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Abstract: Oral drug delivery system is highly accepted amongst patients. In the present era many research and technological advancements are made in novel oral drug delivery. Chewing gum incorporated with various types of active ingredients is one of such example of novel drug delivery. Medicated chewing gum (MCGs) is effective locally as well as systemically in dental caries, smoking cessation, pain, obesity, xerostoma, acidity, allergy, nausea, motion sickness, diabetes, anxiety, dyspepsia, osteoporosis, cough, common cold etc. Medicated chewing gums are used not only for special population groups with swallowing difficulties such as children and the elderly, but also popular amongst the young generation. Thus chewing gum proves to be an excellent drug delivery system for self-medication as it is convenient and can be administered discretely without the aid of water. The present review article has nicely detailed on history, advantages, disadvantages,formulation, manufacturing process, limitation of manufacturing process, factors affecting the release of active substance, quality control tests for chewing gum, significance, stability study and future trends, patent filled on MCGs.The availability of directly compressible co-processed gum material enables rapid, safe and low-cost development of MCG as a drug delivery option. By MCG formulation, revitalization of old products and reformulation of new patented products is possible, to differentiate them from upcoming generics competition in the market.

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OXYGEN NANOBUBBLES AND THEIR APPLICATIONS

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ABSTRACT: Nanobubbles are gas-filled bubbles that spontaneously form at the interface of solid surfaces and aqueous solutions(1) .Nanobubbles can be prepared using various shells, such as phospholipids, polymers, proteins, and surfactants. NBs contain gas cores due to which they are echogenic and can be used as contrast agents for ultrasonic and photoacoustic imaging(2). These bubbles can be engineered in various sizes as vehicles for gas and drug delivery applications with novel properties and flexible structures(1). Hypoxic areas in tumors develop owing to an imbalance of oxygen supply and demand. In tumors, hypoxic regions have shown more resistance to chemotherapy, radiotherapy, and photodynamic therapies(3). The efficacy of photodynamic therapy depends on the effective accumulation of photosensitizer drug in tumors and the availability of oxygen in the tumor to generate reactive oxygen species(4). NBs have been shown to reverse hypoxic conditions, degradation of hypoxia inducible factor 1α protein, and increase tissue oxygen levels. The main purpose of loading NBs with drugs and genes is to minimize the side effects associated with these bioactive substances, along with improving therapeutic efficacy by lowering the effective dosage and minimizing the interference while reaching the target site(2)(5). MNBs can be used for both passive and active targeting. Nanobubble technologies have drawn great attention due to their wide applications in many fields of science and technology, such as water treatment, biomedical engineering, and nanomaterials(3). NBs are reviewed with the focuses on degradation of toxic compounds, water disinfection, and cleaning/defouling of solid surfaces including membrane(5).

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Sustainable strategy(supercritical fluid technology) for nano-in-micro particle engineering for pulmonary delivery

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Abstract: In today's era there is increasing popularity and refinement of inhalation therapy, there has been a huge demand for the design and development of finely tuned inhalable drug particles capable of promising an efficient drug delivery to the lungs with most favourable therapeutic outcomes. To comeup with this demand, novel particle technologies have been arising over the last decade agreeing with the progress of pulmonary therapeutics that were commonly given by injection. Nanotechnology holds a considerable potential role in the development of new release mechanisms of active ingredients to the deep lungs. For an accurate deep lung deposition and effective delivery of nanoparticles, respirable nano-in-micro formulations have been extensively under research. Microparticles with nanoscale features can now be developed, and their functionalities havecontributed to stabilize and improve the efficacy of the particulated dosage form. There are different types of the aerosolizable nano-in-micro particles, as well as their sustainable production and characterization processes as dry powders. The intention to provide a critical insight of the current goals and technologies of particle engineering for the development of pulmonary drug delivery systems with a special emphasis on nanomicro dry powder formulations prepared by supercritical fluid techniques. The merits and limitations of these technologies are debated with reference to their appliance to specific drug and/or excipient materials. Finally, a list of most recent/ongoing clinical trials regarding pulmonary delivery of this type of formulation is described.

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Role of TLR4 receptors in parkinson's Disease

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Abstract: Parkinson's disease (PD) is a progressively debilitating neurodegenerative disease characterized by alpha_-synucleinopathy, which involves all districts of the brain-gut axis, includingthe central, autonomic and enteric nervous systems. Toll-like receptors (TLRs) are pattern recognition receptors which aggrevate an inflammatory response upon the discernment of specific molecular play a critical role in mediating a deleterious immune response to this protein, as well as other inflammatory signals in TLR4 has been described in the brain and seems to regulate some physiological processes,such as neurogenesis. TLR4 has also been reported to play a role during neurodegenerative disorders, including Alzheimer's disease,multiple sclerosis and Parkinson's disease and related α-synucleinopathies. This reviewis focused on reports concerning recent patterns found onforeign organisms and on endogenous damage-related molecules. These receptors play a major role in the activation of microglia, the innate immune cells of the CNS,and are also expressed in peripheral tissues, including blood mononuclear cells and the gut. Aggregated forms of α-synuclein can act as ligands for TLR (particularly TLR4), and hence these receptors may insights into the role and activation mechanisms of TLR4 in the brain, inpathological and physiological conditions, as well as the therapeutic benefit that could derive from TLR4modulation.

Keywords : TLR4, Parkinson's Disease , alpha – synucleinopathy, CNS.

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Analytical approaches for Optimization of microneedle patches

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Abstract: Microneedle patches are used for blood glucose control in patients who have high risk of hypoglycemic condition. The advantages of these patches over other conventional techniques are non-invasive, serve the purpose of effective delivery, pain free, biosafe and patient friendly with availability of self-administration. Classification according to dissolution behaviour is explained here, according to that it has three classes which includes dissolvable, swellable, and degradable patches.The analysis of microneedle patchesis required to ensure safety, potency, and purity of targeted releasing drug.

Analytical methods	**Parameter to be studied**
Physical characterization by fluorescence microscope	For geometric measurements of patches
Scanning electron microscopy	For layer/film thickness
Differential scanning colourimetry (DSC)	Flexibility and temperature fluctuation

Keywords: microneedle patches, dissolvable patches, swellable patches, degradable patches, SEM, DSC

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An Outline on Long Acting Parenterals: Current Scenario and Future Promise for Antiretroviral Therapy

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Abstract : Many chronic diseases require lifetime medication adherence to reduce prevalence of symptoms with time. Hence, regular administration for treatment of such diseases is required which ultimately leads to poor patient compliance. This led to development of LAPs or depot formulations which are known to have sustained or prolonged effect from days to months. This article focuses on one such chronic disease; HIV, that causes irreversible destruction of the immune system. Efforts have been made to design LAPs for HIV which have various benefits over other conventional drugs which includes higher bioavailability, lower dosing frequency, decreased metabolism and targeted drug delivery with minimal side effects. Presently, different long acting ARVs are being studied in phase I / II for both treatment and prevention of HIV infection. The article compiles all major research work towards treatment of AIDS and future attempts for development of more effective controlled delivery of anti-HIV agents.

Keywords: HIV, AIDS, ARV, controlled delivery, depot formulations, sustained effect

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Magnetically triggered drug delivery system and its theranostic values

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19mph109

Abstract: In Conventional dosage form, the treatment is carried out by taking drugs orally or injecting them, so that the drugs are distributed to a large extent throughout the whole human body. This may cause damage to the healthy body cells and tissues, resulting in side effects which may be critical to patients' health. Targeted drug delivery (TDD) is a good solution to this problem, it cannot only cure the disease efficiently, but also reduce the dosage and the side effects. This ability of the TDD is of major relevance in treatment of conditions like cancers, nervous system diseases, sudden sensorineural hearing loss, etc.Drug-delivery systems (DDSs) are nanocarriers designed to guide drug distribution and improve the interaction and release of active compounds in target sites of the body (organs, tissues, or cells) or in microorganisms, retaining the drug locally and decreasing or even totally avoiding toxic effects. Additionally, they prolong the plasmatic life time of the drug, protect theactive compound against chemical or enzymatic post-administration degradation, decrease other side effects, and increase bioavailability. Controlled drug release in nanoparticles (NP) can be triggered by a number of stimuli, either exogenous (variations in temperature, magnetic field, ultrasound intensity, light, or electric pulses) or endogenous (changes in pH, enzyme concentration, or redox gradients). One such popular stimulus is the externally applied magnetic field which gives rise to theMagnetically drug-delivery systems (MDDSs). MDDSs may overcome drug diffusion issues and reduce the systemic distribution of the cytotoxic drug and its associated side effects, as they are guided to the diseased site using a magnet as the driving force. MDDSs can be used in treatment of conditions like cancer, inflammation, etc. and diagnosing diseases like extrapulmonary tuberculosis, atherosclerosis, central nervous system diseases, etc. More improvement and development in magnetically triggered drug delivery is needed. The future perspective in MDDS is control of drug release which can be further enhanced by the useof cross-linked polymers.

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Secondary metabolite profiles of two species of Camellia flowers growing in Kangra region of India and their comparative study

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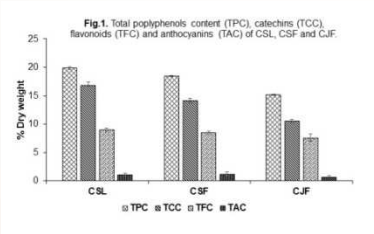
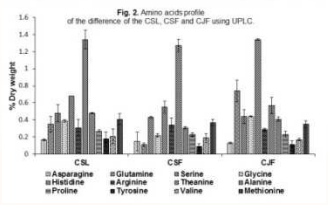
Abstract: Green tea is the choice of beverage world over because of its health benefits.1 Kangra tea based on China hybrid is known for its quality. Flowers and seeds of the plant go waste as tea is clonally propagated.2 Chemical composition of tea is important it influences the taste and quality.3Catechins in tea impart astringency while amino acid gives umami taste. Therefore, to utilize these flowers for making speciality tea along with tea shoots, metabolite profile of Camellia sinensis flowers (CSF), leaves (CSL) and C. japonica flowers (CJF) is compared.

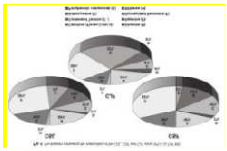
Total polyphenols, flavonoids, catechins and amino acid were estimated on spectrophotometer and UPLC and metabolite profiling by UPLC-Q-TOF-MS.
The quality profile of flower was comparable to the (CSL) (Fig. 1-4). Total polyphenol, flavonoids and catechins content were higher in (CSL) while anthocyanins was higher in (CJF) followed by (CSF) and (CSL). Amino acids were similar and comparable in all the samples, however histidine was higher in CJF while CSF and CSL recorded higher levels of theanine. Fourty four metabolites were identified from CSF, 51 from CJF and 45 from CSL in their metabolome profile.

Consumers are looking for newer range/speciality teas. Accordingly, biochemical content based on TPC, TFC, TCC, amino acid profile, and metabolome were compared to get insight into the composition of water soluble compounds in CSL, CSF, and CJF. The chemical profile and metabolome show that CSF and CJF could be used for either blending with tea shoots or independently processed for specialty tea without compromising on quality.

Keywords: *Camellia sinensis* flowers, *Camellia japonica* flowers, secondary metabolites







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NEWER TARGETS FOR BREAST CANCER

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Abstract: Breast cancer is second most common cause of death among women worldwide and is responsible for elevated death rate.Breast Cancer has ranked no. one cancer amongst Indian females with age adjusted rate as high as 25.8 per 100,000 Women as well as mortality 12.7 per 100,000 women. Breast malignancy occurs when certain cells in breast becomes abnormal and proliferate uncontrollably to form a tumor and cause through manifestation of malignant cells in the breast. Tumor cells are categorized through uncontrolled division, leading to abnormal growth as well as capacity to occupy normal tissue locally. There are various pathways responsible for breast cancer is Ras/raf, PI3K/Akt as well as Wnt pathways. The signaling pathway utilized through EP (prostaglandin E receptor) family of GPCR, their physiological as well as pathological role in carcinogenesis. EP4, as promising newer therapeutic targets for treating breast cancer. Numerous other targets for breast cancer are epidermal growth factor receptor (EGFR), poly (ADP-ribose) polymerase (PARP), and vascular endothelial growth factor (VEGF). EGFR is present in regulation of cell growth in breast cancer. The EP4 inhibitor will protect antitumor activity of natural killer cells from PGE2 mediated Immune suppression. The EP4 target will defeat Immune suppression key to effective tumor control.Related to other cancers; Breast Cancer is on the more improvable completion of the spectrum if diagnosed timely.

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A Review on Nanoemulsion Based Drug Delivery for Curcumin in Cancer Therapy

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Abstract: Nanoemulsions are transparent or translucent oil-in-water (o/w) or water-in-oil droplets with a mean droplet diameter in the range between 100 and 500 nm. Nanoemulsion-based delivery system is superior to conventional topical dosage forms, such as ointment and gels, in several respects. Curcumin is the phytoconstituent which is obtain from turmeric and used as antiseptic, anti-cancer and various other purposes.Cancer is the abnormal growth of the cell proliferating in an uncontrolled way. Cancer therapy has been an issue for several decades. Drugs developed to treat this disease are not always successful or end up failing, mainly due to low solubility, multidrug resistance (MDR), and unspecific toxicity. The efficiency of anticancer drugs is limited by their unsatisfactory properties, such as poor solubility, narrow therapeutic window, and intensive cytotoxicity to normal tissues, which may be the causes of treatment failure in cancer. So Nanoemulsions increase the solubility of drugs exhibiting poor water solubility through entrapment in the core of the nanoemulsion droplets. The purpose of developing the formulation of curcumin lipid nanoemulsion is having the small particle size, highest loading and good physical stability for cancer therapy.

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Investigation of mechanism of action of Canagliflozin against Streptozotocin induced Alzheimer's disease model in rats

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Abstract: Introduction: Worldwide, four million people are affected by Alzheimer's disease disorder. Currently there is nodisease modifying therapy available forAlzheimer's disease. There isneed to find new strategies for treatment of AD. The main objective of this study is to find new targets for treatment. Canagliflozin is SGLT2 inhibitor used to treat T2DM. Epidemiological statistic showspatient having T2DM have more chances to develop AD. The main objective of the present study was to investigate pharmacological effectsand mechanism of Canagliflozin for AD treatment.

Material and methods: AD induced by injecting streptozotocin through intracerebroventricular route. After induction, disease control groups treated with donepezil (5mg/kg) as standard treatment and two doses of Canagliflozin (9 mg/kg, 18 mg/kg) were taken. To evaluate dementia, neurobehavioral tests Y-maze and Morris water maze were performed before induction and after treatment of Canagliflozin. After completion of neurobehavioral parameters, animals were sacrificed, brain was removed, subjected for analysis of biochemical parameters like oxidative stress, anti-inflammatory parameters and histopathology of brain tissue.

Results: In Y-maze test, Canagliflozin treatment increased percentage time spent in novel arm compared to disease control group, improvement was lower than in standard treated group. In water-maze test, Canagliflozin treated group showed improvement in disease but dose dependency was not seen. Results of antioxidant, anti-inflammatory parameters were not significant. Histology of Canagliflozin treated animal showed that treatment with Canagliflozin prevented pyramidal cell loss as observed in disease control group.

Conclusion: Data suggest that Canagliflozin improves disease condition by reducing oxidative stress and inflammatory biomarkers.

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Therapeutic targeting of Toll like receptor 4 by Eugenol: Promising agent for Therapy of neurodegenerative diseases

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Abstract: TLR4 is one of the Toll-like receptors (TLRs), which fall in the family of pattern recognition receptors. TLR4 is a key player in innate immunity and involved in the pathogenesis of various neurodegenerative diseases. Eugenol is a dietary phytochemical with potent anti-inflammatory and anti-oxidant activities. The present study aimed to investigate neuroprotective role of eugenol against experimental models of neurodegenerative diseases (Parkinson's disease and Traumatic brain injury). To study the interaction of eugenol with TLR4, docking studies were also performed using the Surflex–Dock module of SYBYLX software by using the crystal structure of hMD-2 (PDB ID: 2E59). Male Sprague drawly rats were administered orally with Eugenol (100 mg/Kg) or vehicle for seven consecutive days. On the seventh day, rats were subjected to weight-drop contusion injury. In other set of study, Eugenol (100 mg/kg) was administered orally once a day for seven consecutive days. From 3rd day MPTP (3 mg/kg, i.p.) was co-administered with eugenol for five consecutive days. Finally, locomotor activity and motor coordination were estimated in all the animals using actophotometer and rotarod, respectively. Result of Insilco docking studies showed that the docking score of eugenol with TLR4 is 4.75. Results also show that the TBI and MPTP administration resulted in impairment in motor coordination and locomotor activity. However, Eugenol pretreatment ameliorated the behavioral consequences of MPTP administration as well as trauma. Thus eugenol is effective against traumatic brain injury and Parkinson's disease. This neuroprotective effect of eugenol might be due to its inhibitory activity on TLR4.

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Chemistry of Non-NAD$^+$PARP1 Inhibitors as Anti-tumor Agents

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Abstract: PARPs are an important family of 17 nucleoproteins marked by a particular catalytic site that uses NAD$^+$ as a cofactor to transfer an ADP-ribose group to a different acceptor protein. PARP1 is the most abundant enzyme of the PARP family, also referred as “Guardian angel of DNA”. PARP1 plays diversified biological functions such as synthetic lethality, repair of DNA, apoptosis, necrosis, binding of histones, etc.PARP plays a key role in the mechanistic pathway of base excision repair (BER), does parylation of the target pathway and promotes cell apoptosis at high DNA destruction rates.It has already been shown that PARP1 inhibitors have the ability to treat different types of cancer, namely prostate, colorectal and pancreatic tumors, beyond BRCA1/2 ovarian cancer. As NAD$^+$is found in abundance in human body and is a natural substrate for many enzymes, NAD$^+$analogues seem to possess various off-target side effects due to their interference in many other important metabolic pathways. Another specific and alternate mechanism to block PARP1 is through histone H4 dependent pathway. Based on it, anovel non-NAD$^+$lead molecule 5F02 has shown much better activity in human prostate cancer cell lines than the marketed NAD analogue, Olaparib. This review provides insight into the recent development of new lead structures as non-NAD analogues inPARP1 inhibitors, their SAR, an overview of *in-vitro*and *in-vivo*screening methods, current challenges, and opinion on the future design of more selective and effective PARP1 inhibitors.

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Antioxidant status in Silica Nanoparticles (SiNPs) induced Neurotoxicity

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ABSTRACT: Silica nanoparticles (SiNPS) are found to be toxic element during excessive exposure (Peters et al., 2012). The main routes of exposure are inhalation, ingestion and other environment factors (Scott, 2016). Moreover, exposure of SiNPs is an important cause for neurodegeneration (Liao et al., 2015). We have attempted to investigate the effect of SiNPs toxicity in the rat's central nervous system.

In the present study, 40 and 80 mg SiNPs were exposed to rats for eight weeks. At the end of the exposure period, the experimental rats were sacrificed by anaesthetic overdose, brain was removed for the biochemical investigations like, lipid peroxide levels (LPO), protein carbonyl content (PC), superoxide dismutase (SOD), catalase (CAT), glutathione peroxidase (GPx) and glutathione (GSH).
Results of the present study demonstrates that SiNPs intoxicated rats were found to have increased LPO and PC, while the antioxidant status of SOD, CAT, GPX and GSH were found to be decreased in the brain when compared with the control rats.
On the basis of results it may be concluded that the oxidative stress markers increased in the intoxicated rats and the antioxidant therapy may be a remedy for SiNPs exposed population. Furthermore, it may be recommended for clinical trials.

Keywords: Silica nanoparticles, Neurodegeneration, Superoxide dismutase, Catalase, Glutathione peroxidise

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SILICA NANOPARTICLE ALTERS REPRODUCTIVE HORMONES IN MALE RATS

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ABSTRACT: Silica nanoparticles (SiNPs) are found to be toxic during excessive exposure for both human and animals (Fan et al., (2006). The main routes of exposure are air, drinking water and other environment factors (Leung et al., 2012). It is reported that SiNPsdecreased the sperm number and sperm motility rate and further it is reported that silica caused the sperm malformation, and apoptosis in the testicle spermatogenic cells in rats (Ying et al., 2014). In aim of the present study is to evaluate deterioration in male reproductive hormones in SiNPs exposed rats

In the present study, 40 and 80 mg SiNPs were exposed to rats for eight weeks. At the end of the exposure period serum were removed from the blood for the investigation of reproductive hormones such as Folicle stimulating Hormones (FSH), Leutinizing Hormones (LH), Testosterone (TT) and Prolactin (PR) in both control and experimental rats.

In the present study it was found that LH, FSH, Testosterone and Prolactin values significantly alters SiNPs exposed groups when compared with control groups. We also found that epididymal sperm count was decreased significantly in the experimental groups.

On the basis of results it may be concluded that the interperitoneal injection of SiNPs alters the male reproductive hormones, which further deteriorate the spermatogenesis.

Keywords: Silica nanoparticles, Folicle stimulating Hormones, Leutinizing Hormones, Prolactin, Testosterone.

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CLINICAL STUDY ON DRUG UTILIZATION PATTERN AND EFFECTIVENESS OF PALLIATIVE CHEMOTHERAPEUTIC TREATMENT IN ORAL CANCER PATIENTS

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Abstract: Oral squamous cell carcinoma (OSCC) is the infirmity wherein the incidence rate of metastatic recurrence is about 50-60% in patients with former history of oral cancer. The main objective of the study was to evaluate the drug utilization pattern and effectiveness of the palliative chemotherapy in cases of OSCC.Thisprospective longitudinal study was approved ethically by IRB at KCHRC and was conducted in the palliative care department to observe the patient characteristics, their treatment profile, recurrence profile, palliative treatment details and their quality of life. Data collection was done by paper-based case record form and Quality of life questionnaire.Total 104 patients were enrolled and 83 patients completed the follow up. In the study incidence ratio for male to female was 15:1, median was age 57.50±12.54 with 18.39 % of family history of cancer. The patients of recurrent disease were treated with tailored dose of platinum compounds either alone or in combination with taxanes or anti-metabolites. The results of paired t-Test for quality of life questionnaire tool revealed that the palliative chemotherapy was efficient for management of physical, emotional, social and other disease related factors ($p \leq 0.05$). The incidence of grade II and grade III toxicity was observed in total 41 patients. TPF therapy was found to associated poor QoL outcomes while paclitaxel in combination carboplatin yielded best QoL outcomes. Tailored drug therapy approach for palliative chemotherapy was potential intervention for terminal oral cancer patients with less incidence of toxicitywasconcluded.

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Identification of 16 degradation products and characterization of major degradation product in Avanafil using HPLC, LC-MS and NMR.

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Abstract: Avanafil (AV), a phosphodiesterase type 5 inhibitor drug used for the treatment of erectly dysfunction was subjected to forced degradation studies as per ICH guideline Q1A (R2). The present report emphasis on identification of degradation products and degradation pathway of Avanafil (AV) in different degradation conditions. Sixteen degradation products (AV I- AV VI)were identifiedfrom different degradation conditions and these were identified using a simple, isocratic and mass compatible liquid chromatography method with PDA detector. The degradation product structures were identified by mass chromatography. One major hydrolysis degradation product was isolated using column chromatography and concentrated byrota evaporator. Further, the collected solid degradation product was characterized using UV, Mass, ^{1}H and C^{12} NMR spectroscopy. Structure of degradation products were confirmed from fragmentation pattern obtained by LC-MS/MS and further plausible degradation mechanism for each stress conditions has been proposed. Comprehensive stress study reveals that AV is more prone to degrades in light, temperature and moisture, hence AV requires proper storage condition temperature below 25 °C with protection to light and moisture. In detailed, LC-MS/MS compatible AV degradation study is fully validated as per ICH guideline, hence can further beneficial for pharmacokinetic study and toxicity study.

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DEVLOPMENT, OPTIMIZATION AND EVALUATION OF BUCCAL FILM FOR HYPERTENSION OF BCS CLASS 1 DRUG

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Abstract: According to the Indian statistics of 2015 29.8% patients are suffering from hypertension. Hypertension is a long-term disease commonly called as High Blood Pressure. It is a medical condition in which the force of blood is against the arterywall is too high. The normal range of the blood pressure is 140/90. Tablets,Suspension,and Intravenous route of delivery prevail in the market but their disadvantageof patient compliance is the major issue.Buccal films are the novel approach and it also resolves the issue of patient compliance. Buccal mucosa eliminates the first pass metabolism thus the formulation directly enters the systemic circulation and gives fastest onset of action. Other than the fastest onset of action there are many advantages of buccal film like increase the rate of dissolution, enhanced efficacy, and highly stable. The challenge of gastric trouble is also resolved in this formulation.Buccal films can be prepared through multiple techniques such as Solid Dispersion, Hot Melt Extrusion, Rolling Method and Film Casting Method. Sildenafil citrate is a selective inhibitor of phosphodiesterase type 5 enzyme. The purpose of the drug when found was hypertension but it is extensively used in market for treating erectile dysfunction. The bioavailability of the drug is 40% when administered orally in the form of tablet (20mg). The trial batches will be prepared by Solvent Casting Method. The trials will be taken by varying the concentration of polymer and plasticizer, and then will be evaluated.

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AN INNOVATIVE APPROACHES FOR SPECIFIC TUMOR TARGETING

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Abstract: Tumor formation and its treatment is one of the most life threatening problem now a days, its prevention and inhibition is also challenging task.Tumor has characteristic of metastasis by that it can spread to other body parts from the origin, for inhibition of it killing of tumor original cell and spread cell is required that done by the chemotherapeutic agent, which has cytotoxic effect. Most common problem with chemotherapeutic agent is that it can not differentiate normal and tumor cell and give cytotoxic effect to normal cell also. To address this problem we have to target chemotherapeutic agent to specific tumor cell so it can kill only the tumor cell and give minimal adverse effect. For the targeting chemotherapeutic agent to tumor cell there are so many different approaches like prodrug, change in drug delivery system and use of nanotechnology. Here I come up with some innovative drug delivery approaches for specific tumor targeting to get good therapeutic effect with minimal adverse effect.

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HYBRID DRUG NANOCRYSTAL

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Abstract: Nanocrystals have drawn increasing interest in pharmaceutical industry because of ability to improve dissolution of poorly water soluble drug in nanometer range. Nanocrystallization is an approach to enhance the dissolution of drugs crystal. Due to size and high surface area to volume ratio, nanocrystal can increase the saturation solubility of drug and dissolution rate of drugs particles. Nanocrystal are crystalline drugs particles with size generally smaller than 1 µm. Transfer of material into nanodimension changes their physical properties which were used in pharmaceutic to develop innovative formulation for poorly soluble drugs. Nanocrystal can be produced by top-down and bottom-up technologies and have been explored for a variety of therapeutic applications like oral, dermal, pulmonary, systemic administration and targeted drug delivery and intraperitoneal chemotherapy . The dying crystal phenomenon inspired the development of hybrid nanocrystal for concurrent therapy and bioimaging by physically embedding imaging agent (e.g. fluorophores, radionucleotides, and contrast metals) into the crystal lattice. A hybrid nanocrystal system may be composed of a drug, an imaging agent, a ligand, and or biocompatible polymer. Nanocrystal also offer advantages of long term durability in body for interacting with biological tissues and cell. Till date, many nanocrystal drug formulations are currently marketed for either parenteral or oral administration.This review introduces the hybrid nanocrystal technique, including the theoretical concepts, properties, nanocrystal as drug delivery system, preparation, nanocrystal product for oral administration approved by the FDA and applications.

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Synthesis andBioevaluation of New 1, 2, 3-Triazole Incorporated Bis-Indolylmethanes

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Abstract: Bis-indolylmethane(BIM) is the key structural motif abundantly found in natural products.Syntheticderivatives of BIM exhibits wide range of important biological activities such asantitubercular,anticancer, anti-tumorigenic, anti-inflammatory,antimicrobial,antifungal, antioxidantand cytotoxic activities [1].Therefore,BIM scaffold is extensively used as building block in rationale of drug design.Conjugation of functional molecules through 1,2,3-triazole has received great attention in drug discovery as 1,2,3-triazole structural motif is a neoclassical bioisostere of amide and found in approved drugs[2]. Moreover, 1,2,3-triazole with amide linkage are reported to possess anticancer, antifungal, anti-tubercular,antioxidant activities. Considering the pharmacological importance and in continuation of our interest in the development of new hybrid molecules that comprises more than two pharmacophore in a single molecule with an intention to enhance the efficacy and bring synergy in hybrids.In accordance with the molecular hybridization approach,we have designed and synthesized highly functionalized1,2,3-triazole bearing *N*-phenacylacetamide incorporated bis-indolylmethanes by usingcopper (I)-catalyzed azide–alkyne cycloaddition (CuAAC) reaction[3].The newly synthesized conjugates have been screened for their bioevaluation study and will be presented.

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Hunting for potent anti-tubercular Inhibitors: virtually4-(3-(4-substitutedpiperazin-1-yl)quinoxalin-2-yl)naphthalen-1-ol analogues

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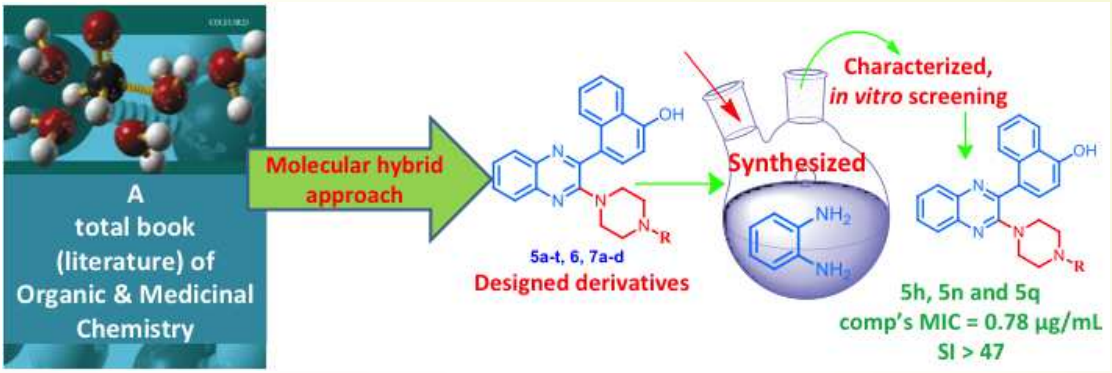
Abstract: A series of twenty-fivenovel 4-(3-(4-substitutedpiperazin-1-yl)quinoxalin-2-yl)naphthalen-1-ol analogues were synthesised, characterized and screened Naidu et al [1,2] for their *in vitro* anti-tubercular activity against *Mycobacterium tuberculosis* H37Rv strain. These compounds exhibited minimum inhibitory concentration between 0.78 – ≤50 µg/mL. Among these derivatives, compounds **5a, 5b, 5f, 5m, 5p** and **5r (**MIC 3.125 µg/mL) displayed moderate activity, whereas compounds **5c, 5d, 5g, 5l** and **5o** (MIC 1.56 µg/mL) showed good anti-tubercular activity and compounds **5h, 5n** and **5q** (MIC 0.78 µg/mL) exhibited excellent anti-tubercular activity. In addition, MTT assay was performed on the active analogues of the series against mouse macrophage cells to assess the cytotoxic effect of the newly synthesized compounds and selectivity index of the compounds was established; Collins et al [3]. Selectivity index values of the most active compounds is > 47 indicating suitability of compounds for further potential anti-tubercular drug development.



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Exploring NLC based nanosuspension of multikinase inhibitor for the treatment of head & neck cancer.

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ABSTRACT: The rising incidence of head and neck cancer and drawbacks of currently used therapeutic strategies such as salvage surgery followed by adjuvant chemo- or radiotherapy have encouraged pursuits for better therapeutic approaches. Many chemotherapeutic agents are used such as multikinase inhibitors, monoclonal antibodies, antimicrotubule agents etc. from which multikinase inhibitors have emerged that have shown convincing efficacy against such tumors. This include cabozantinib, imatinib, sorafenib, sunitinib, & vandetinib from which sorafenib inhibits overexpressed tyrosine kinase receptors in head & neck cancer by blocking signals within the tumor cells and tumor vasculature. It comes under BCS class -2 and shows decreased bioavailability at the site of tumor cells. The NLCs of multikinase inhibitor increases solubility & permeability, enhance storage stability & reduce adverse effects with targeted delivery. The NLC based nanosuspension could successfully enhances solubility, give sustained release drug delivery due to which dose reduction is possible. Thus, multikinase inhibitor-loaded NLC based nanosuspension increases the bioavailability & therapeutic efficacy against head & neck cancer. This review enlightened the challenges, opportunities & application of NLC based nanosuspension of multikinase inhibitor for the treatment of head & neck cancer.

Keywords: NLC, multikinase inhibitor, head & neck cancer.

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APPROVED DRUGS PRODUCTS WITH THERAPEUTIC EQUIVALENCE EVALUATION – A REVIEW

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ABSTRACT: During the 1970s, to overcome drug costs, every state adopted laws that brought towards the replacement of drug products. So the approach of Positive and Negative formulary had to be prepared by the FDA, so it became superficial that FDA could not serve the need of preparing both the formularies. So in the year 1978, the commissioner of Food and Drug Administration sent a letter to the officials of each state to provide a list of all prescription drug products that are approved by FDA. So finally on 31st October 1980, the first edition of the orange book was published in the federal register which was termed as Orange Book (Approved Drug products with therapeutic equivalence). Each year FDA publishes updated and corrected edition of Orange Book,and the latest edition of Orange Book was published on January 2019 as 39th Edition. Orange Book generally categories drug products with multi-source and single-source drug products. Classification of all approved drug is assigned with specific therapeutic codes, i.e. A code and B code according to the equivalence of a drug with other pharmaceutical equivalent products and not equivalent with other pharmaceutical equivalent product respectively. The prime objective of the Orange Book is that it identifies the drug products by safety and efficacy purpose by FDA. It also helps health care professionals, physicians, and industrialist under various categories. The cumulative updates of Orange Book are published every month with corrections and updates of newly approved drugs, patent and exclusivity data with applicant name changes.

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Exploring nanowafer for opthalmic drug delivery

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ABSTRACT: Dry eye syndrome is the multifactorial the most common disease spreading in the worldwide. Dry eye syndrome is mainly caused by the lack or insufficient moisture and lubrication on the anterior portion of the eye which may cause irritation, burning sensation, itchy eyes, fatigued eyes, sore eye, dryness sensation, aching sensation etc. It involves both metabolic and immune deregulation. For this disease eye drops and many conventional drug delivery systems are used for the treatment of dry eye syndrome but in case of conventional drug it did not gave the more therapeutic effect and also less bioavailability. To improve the convenience and efficacy, cyclosporine loaded nanowafer are developed. Nanowafer are the small disc like structure or thin rectangular membrane drug loaded reservoir. Through which drug releases for the sustained period of time and gives the more therapeutic and bioavailability compared to the conventional drug delivery. Nanowafer are applied by the help of the tip of the finger to the anterior part or surface of the eye and it is applied as such that the reservoir or drug loaded are direct contact with the surface of the eyes and at last if get dissolved on the surface of the eyes and fades away.

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DEVELOPMENT OF GEL-IN-CREAM COSMECEUTICAL FORMULATION FOR THE TREATMENT OF ROSACEA

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ABSTRACT: Rosacea is a chronic dermal condition with the unknown root cause, causing the redness, small papules, pustules and nodules in the centre of the face.[1] The more likely population to be affected is between the ages of 30-60 with the fair skin.[3] As age increase the level of hyaluronic acid and the collagen starts declining, which makes the skin weak and prone to the disease related to it. [1][2] Majorly the factors that affect the skin aging are the same that of the rosacea they are co-linked with each other. [2] Dermocosmetics have created their own space in the dermatology as they, offer support to control various skin phenotypes and skin disease. There are many marketed semisolid topical formulation available such as gel, cream, lotions for the treatment. [4] Gel-in-cream is an innovative concept which subside the basic disadvantages of local irritancy and inflammation of other marketed topical formulation. Incorporation of gel into cream reduces the local irritancy and provides the hydration to the infected skin. In the present research work is on the Development of gel-in-cream cosmeceutical formulation for the treatment of Rosacea. Actives act as the active ingredient in cosmetics; in this cosmetic formulation two actives are used, derivatives of Hyaluronic acid and Colloidal oatmeal have shown their prominent result in treating the sensitive skin. Disodium Acetyl Glucosamide hydrates the skin 1000 times and Colloidal Oatmeal provides good anti-inflammatory antiaging and moisturizing effect when applied. The formulation is prepared by preparing the gel and then addition of the gel into cream. Qualitative evaluation of the formulation can be done through physical attributes. Gel-in-cream formulation will show the promising approach to treat rosacea.

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European Union's new Medical Device Regulation: same arena with different modulation

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ABSTRACT: Medical devices include different products and their importance in the healthcare industry is truly remarkable. Main problems for group developing and manufacturing medical devices is that current regulatory of necessity must be updated according to regulatory requirements and must be done during the manufacturing process. The European medical device industry accounts for around a third of world production. The Medical Device Directives are a "new approach" directive on the safety and performance of medical devices that have been harmonized in the EU in the 1990s. But the new regulation EU Medical Device Regulation (EU MDR), which took effect in 2017, will be fully applicable in May 2020 for medical devices and May 2022 for in vitro diagnostic medical devices. It is four times longer than its predecessor and has significant changes in the wording used. Companies will need to rationalize their portfolios and conduct global impact assessments so they can implement the changes necessary to remain compliant. The aim of the new regulation is to address some inherent weaknesses in the old directives as well as the swift evolution of science and technology in the field of medical devices. Manufacturers will need to provide more in-depth clinical data which proves safety and performance claims and have tighter equivalency standards. In the near future, the innovative products could fill the gaps left by drugs for a synergic therapeutic action, which could benefit the European and worldwide population. If this is not allowed to happen, it will be an important opportunity lost.

Keywords: Medical Device Regulation, Healthcare, Clinical Investigation, Regulatory framework

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P-183

Bioanalysis of Monoclonal Antibodies

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ABSTRACT: Monoclonal antibodies are protein molecules of therapeutic importance preparedfrom a single clone of plasma cells that arewidely inuse in today's times for targeted therapy mainly duetotheir long serum half-life and potency. Bioanalysis of monoclonal antibodies refers to the quantitative measurement of the same in biological fluids such as plasma, serum, urine, etc. the two main methods employed to conduct bioanalysis are ligand binding assays and LC-MS/MS. While, the principles employed by these methods are different from eachother and they have their respective pros and cons,these methods still remain the most used methods for bioanalysis. This poster covers the basic aspects of monoclonalantibodies and provides a brief description about the steps involved in the bioanalytical methods, namely, LC-MS/MS and ligand binding assays.

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SUPERCRITICAL FLUID CHROMATOGRAPHY IN CLINICAL CHEMISTRY

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ABSTRACT: Supercritical fluid chromatography (SFC) is a separation technique for resolving complex mixtures of non-volatile, or thermally labile components. SFC is a subset of high-performance liquid chromatography (HPLC), sharing much of the same hardware and methodology. SFC is most often a normal phase technique but with vastly superior characteristics compared to normal phase HPLC. Supercritical fluid extraction using carbon dioxide (CO_2) has been recognized as a green technology. Modern SFC is performed almost entirely on packed columns. Packed-column supercritical fluid chromatography (pSFC) is a fast separation technique that combines the properties of HPLC and GC. Coupling of SFC with different detectors allows for straightforward use in bioanalysis. Some of the emerging applications of SFC in pharmaceuticals, such as particle design, drug solubilization, inclusion complex, polymer impregnation, polymorphism, drug extraction process, and for lipid analysis. It is increasingly used for analytical, semi-preparative and preparative purification of chiral compounds, including production of enantiomers that are mainly encountered during drug development. SFC can be used as an alternative to HPLC for many drug substances, so it is gaining popularity in the pharmaceutical industry. The main advantages of SFC in separating chiral pharmaceuticals are: high speed, short analysis time, limited environmental impact and high efficiency. The reduction in the use of organic solvents has cost, health, and safety benefits. Due to these advantages, SFC fulfills all the requirements of Green Analytical Chemistry approaches.

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P-185

Synthesis and anion inclusion applications of sugar-amino acid based macrocycles

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ABSTRACT: In anion complexation chemistry, carboxylate anion complexation with supramolecular structure is currently attracting interest of researchers due to their chemical as well as biological roles, such as carboxylate anion in carboxypeptidase A, carboxylate anion in biological activity of vancomycin family of antibiotics and enzyme-substrate interactions,etc.In this endeavour, we have synthesizedmacrocyclic compounds using 2,6-anhydro-glucoheptitol, glycineand dicarboxylic acid linkers, *viz.* succinic acid and pyridine dicarboxylic acid. The anion inclusion capabilities of synthesizedmacrocyclic compounds have been studied using boc-GlyCOO$^-$anion by^{1}H NMR titration studies in $CDCl_3$solvent. The macrocyclic compound **1** and **II**both have shown strong binding affinity towards carboxylate anion present in TBA salt of *N*-boc-glycine. The detailed synthetic protocol and binding data will be discussed during poster presentation.

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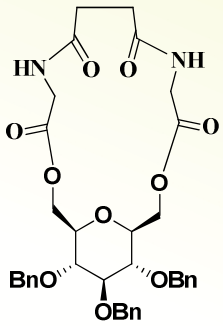
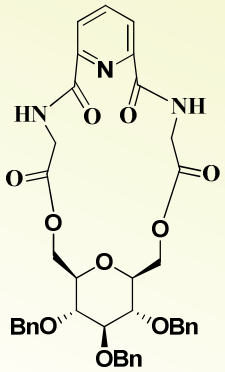


Macrocycle I



Macrocycle II

Acknowledgement- We are thankful to University of Delhi for providing financial support under DU-DST Purse Grant & Scheme to Strengthen Research and Development, and to CIF-USIC of the University for providing Mass and NMR recording facility. HS thanks CSIR (New Delhi) for the award of Junior Research Fellowship.

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P-186

Isolation and characterization of phytochemicals from*CapparisZeylanica*Linn. roots extract

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Abstract: In this study, we isolated, identified and characterized the phytoconstituents of *CapparisZeylanica*Linn. alcoholic root extract. The extract was analyzed by GC-MS between 0 to 30 min time intervals. The extract was further eluted in column using petroleum-ether- chloroform and chloroform - ethanol at different combinations. Identity of the constituents isolated was confirmed by comparing data of physicochemical and spectral characteristics (M.P., UV, IR, Mass, 1H and 13C NMR spectra) with the reported data in literature. Five compounds were obtained by column chromatography of the extract are β-amyrin, stachydrine, stigmasterol, decanoic acid (Capric acid) and 4-hydroxy benzoic acid. GC-MS study also revealed several biologically active compounds. Based on the results obtained, it is possible to conclude that ethanolic extract of *Cappariszeylanica*roots have biologically active compounds which would be responsible for the biological activity.

Key words: Triterpenoid; Stachydrine; *CapparisZeylanica*; n-Decanoic acid.

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Chemo-enzymatic route to novel bicyclic homo-nucleosides

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Abstract: Bicyclic nucleosides and their analogues are of much importance due to their immense potential as key intermediates for the development of antisense and/or antigene oligonucleotides[1,2]. These nucleoside monomers possess constrained sugar puckering, which enable them to mimic a DNA or RNA type furanose ring conformation that regulates targeted gene expression. These sugar modified nucleosides have emerged as one of the most promising modification in development monomer for antisense approach and gene therapy oligonucleotides due to their restricted conformational structures[3,4,5].

Henceforth, in the present work we have designed and carried out easy access to conformationally restricted bicyclic5'-homonucleosides (**Figure 1**). The structure of homonucleosides was confirmed by the single crystal X-ray diffraction analysis which depicted the conformation of the sugar ring and the orientation of the 5'-hydroxylmethyl group. Detailed results will be presented during poster presentation.

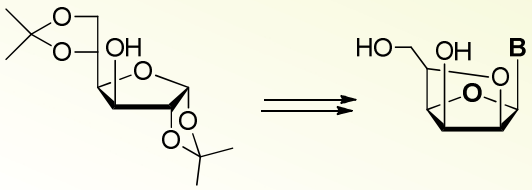

Figure 1.5′-homonucleosidesfrom diacetone D-glucose.

Acknowledgement: We are thankful to University of Delhi for providing financial support under DU-DST Purse Grant & Scheme to Strengthen Research and Development, and to CIF-USIC of the University for providing Mass and NMR recording facility. SK thanks CSIR (New Delhi) for the award of CSIR-SPM fellowship.

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Efficient route for the synthesis of highly substituted chromanes

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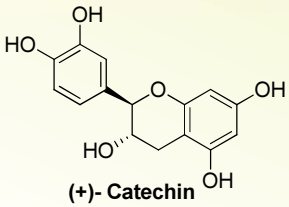
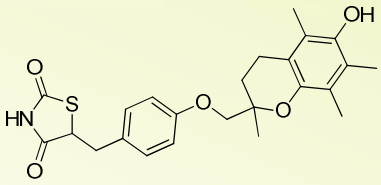
Abstract: Chromanes are known to exhibit various biological and pharmacological activities such as anti-rhinovirus, antiplasmodial, antidiabetic, anticancer, anti-HIV, antibacterial and antifungal activities. Chromane core makes structural framework of complex compounds, including Vitamin E and other pharmaceutical drugs, such as ormeloxifene, troglitazone, nebivolol, etc. Due to the biological importance, effort have been made by researchers for developing efficient synthetic methods to access chromanes.

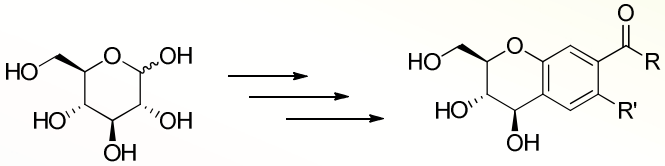


(+)- Catechin



Troglitazone

In most of the synthetic strategies, reaction of salicylaldehyde and enolates or their equivalents obtained from aryl methyl ketones has been utilized for synthesizing chromane derivatives. In all reported methods construction of pyran ring system has been carried out around the aromatic ring.
We have developed a new strategy for the synthesis of highly functionalised chromane derivatives from natural and readily available D-glucose *via* metal catalyzed oxidative C-H activation and subsequent cyclization. The aromatic ring has been constructed at 1,2-position of glucopyranose ring. Details of the synthesis will be presented in the poster.



1
D-Glucose

2-12
Sugar derived chromanes

Acknowledgements: We are thankful to University of Delhi for providing financial support under DU-DST Purse Grant & Scheme to Strengthen Research and Development, and to CIF-USIC of the University for providing Mass and NMR recording facility. BS is thankful to Deshbandhu College, University of Delhi for providing leave to pursue PhD under career development program.

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INVOLVEMENT OF TOLL LIKE RECEPTORS IN TRAUMATIC BRAIN INJURY

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Abstract: Death due to traumatic injury or intracranial injury is one of the most silent epidemic, which is growing wide spread. It is a disease which cannot be controlled by any vaccine or premedication, but only by preventing oneself from facing any kind of injury. Scientists have been working on the various pathways which are being involved in the progression of the Traumatic Brain Injury led by PRP receptor family. Traumatic brain injury as a disease needs an immediate attention for the treatment, as more time the immune system of the body gets, more could be the detoriation inside the Brain. Different parts of the brain including Blood brain barrier, neurons, microglia, endothelial cells, and astrocytes are responsible for the damaging the brain in different manner. Toll like receptors (TLR) from the PRP receptor family has an active signalling pathway which initiates the inflammatory response of the immune system following any brain tissue damage and neurological dysfunction. Hence TLR associated downstream cascade activation pathways is a potential target for treatment of Traumatic Brain Injury.

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THIOLATED CHITOSAN: A NOVEL MUCOADHESIVE POLYMER.

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Abstract: The mucoadhesive drug delivery system is a popular novel drug delivery system because of permeability of mucous membrane allowing rapid uptake of drug and avoiding first pass metabolism. Mucoadhesion can be defined as a state in which two components of which one is of biological origin are held together for extended period of time. Mucoadhesion term is used when a bond is formed with mucosal membrane. Mucoadhesive properties can be explained by interactions with glycoprotein on the mucus, based mainly on noncovalent bonds such as ionic interactions, hydrogen bonds and van der waal forces. The drugs which have a local action or those which have maximum absorption in GIT requires increase duration of stay in GIT. Novel mucoadhesive polymers generally includes modifications of existing one, which includes lectins, thiolated polymers (thiomers), poloxamer pluronics and its combinations.(1) chitosan doesn't bear any thiol group in its structural skeleton,but the same structure provides opportunity to modify it when this novel polymer is thiolated it offers many benefits ranging from imparting mucoadhesive property to permeation enhancement of proteins. Thiolated chitosan is unique because it is only cationic thiomer providing mucoadhesive property . Chitosan is widely used in biomedical and polymer science because of its versatility but major drawback is its solubility constraints. It is only soluble in acidic medium (below pH 6) because it is cationic exchange proton in acidic medium which is not available in basic or neutral medium to overcome this drawback, chitosan can undergo chemical modification.Various derivatives of chitosan like carboxylated, thiolated,acylated and conjugates offers the best way to overcome the solubility problem.(2)The strong cohesive properties of thiolated chitosans make them highly suitable excipients for controlled drug release dosage forms. Moreover, solutions of thiolated chitosans display in situ g(4)Thiolted chitosans are polymers for targeted drug delivery mainly by preparation of nanocarrier such as niosomes, lipososmes, nanoparticles, carbon nanotubes having a wide range of application as follows thermosensitive hydrogel based on thiolated chitosan, as coating polymer for stents, matrix tablets for controlled drug delivery.(8)

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P-191

Successive Extraction And Preliminary Phytochemical Testing of Different Extract of *Lepidium Sativum* Linn. Seeds

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Abstract: Herbal medicines are in nice demand within the developed additionally as developing countries for primary aid due to their wide biological and medicative activities, higher safety margins, and lesser prices. *Lepidium sativum* Linn. (Brassicaceae) is annual herb regionally referred to as halon in India, however, usually referred to as garden cress. *L. sativum* is a fast growing edible plant. Seeds, roots, and leaves of garden cress have economic importance; however, the crop is especially cultivated for seeds. Succesive solvent extraction of seeds with n-hexane, chloroform, ethyl acetate and methanol was done by using soxhlet apparatus. Extracts from different solvents were subjected to various phytochemical tests to detect phytoconstituents like alkaloids, amino acids, flavanoids, tannins, proteins, steroids, terpenoids, carbohydrates and glycosides. For detection of alkaloids- Dragendorff's, Mayer's, Wagner's and Hager's tests and for amino acids- Millon's and Ninhydrin tests were performed. For flavanoids- Shinoda, alkaline reagent, Zinc hydrochloride tests were performed. For tannins- ferric chloride, phenazone, gelatin tests were performed. For proteins- biuret, hydrolysis and trichloroacetic acid tests and for steroids and triterpenoids- libermann- burchard and salkowski tests were performed. For cardohydrates- molish's, fehling and benedict tests were performed for each extract. Screening of n-hexane extract indicated the presence of amino acid and terpenoids, chloroform extract indicated presence of carbohydrate, glycoside and steroids. Ethyl acetate extract indicated presence of amino acid and terpenoids, methanol extract indicated presence of alkaloid, amino acid, tannin, terpenoid and flavanoids. This information can be used further as identification of specific constituent responsible for particular pharmacological activity.

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Convenient Synthesis of Sugar based Chromanes

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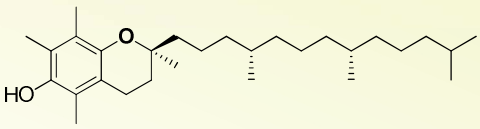
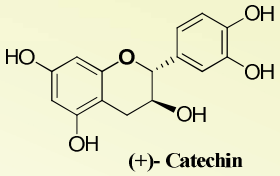
Abstract: Chromanes[1] are associated with a broad range of biological and pharmaceutical activities such as anticancer,[2] antioxidant,[3] antidiabetic,[4] antihypertensive,[5] etc. Chromane core makes structural framework of complex compounds, including α-tocopherol, (+)-catechin, and pharmaceutical drugs, such as troglitazone, ormeloxifene, nebivolol, etc. Due to the biological importance of chromanes, efforts have been made to develop an efficient and selective synthetic method to afford compounds of this class.[6]

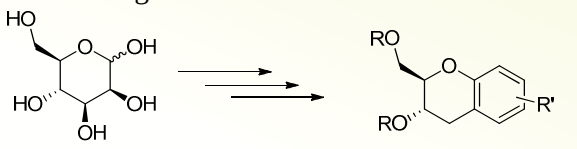


α- Tocopherol



(+)- Catechin

In the reported methods so far, synthesis of chromanes have been carried out by taking pertinently functionalized aromatic moiety as starting compound in order to annulate the pyran system.[7] Fusion of an aromatic system with pyranosugar to synthesize chromanes is still an arduous task in synthetic organic chemistry. In this endeavour, we have developed a new strategy for the formation of chromane core using metal catalyzed oxidative C-H activation followed by subsequent cyclization / dehydrogenation from *C*-1substituted glucal which is derived from mannose.[8]



D-Mannose Substituted Chromanes

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Study of L-asparaginase activity from marine bacterium *Bacillus* sp. for potential application in pharmaceutical industry

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Abstract: Marine bacteria are the sources of several important microbial metabolites and enzymes. Althogh the same genera of bacteria may be isolated from terrestrial source also, the bacteria of marine origin have different, superior or novel properties. The isolate *Bacillus licheniformis* RS2 was isolated from sea water directly, without enrichment in any media or screening for any particular property. After several subcultures and maintenance as pure culture it was studied for some properties. It was found to consistently produce extracellular polymeric substance. The polymer was viscous and a potential biomaterial. The viscosity of the polymer was studied using viscometer. On further study the bacterium was found to be efficient in utilization of amino acids such as glutamine and asparagine as growth substrate. The enzyme of bacterial cell catalyze the hydrolytic reaction of such amino acids into deaminated form and ammonia [1]. The *Bacillus* isolate was able to utilize amino acids and the major extracellular product was ammonia. The activity was seen at different pH and the polymer formation also was marked in high pH condition. Anti-tumour of property of L-asparaginase was recognized years ago when it was discovered that the regression of lympho sarcoma transplants in mice treated with guinea pig serum was due to nutritional dependence of the malignant cells on the exogenous L-asparagine and evidence that L-asparaginase in the serum was the anti-tumor factor. Thereafter asparginase is used in tumour treatment [2]. First microbial l-asparaginase was commercially produced from *E. coli* though asparaginase is broadly distributed among the plants, animals, microorganisms. Due to the difficult extraction procedure for plant and animal asparaginase, potential microbial sources are better for large-scale production microorganisms have been proved to be very efficient and inexpensive sources of L-asparaginase. Large number of bacteria, fungi, yeast, actinomycetes and algae are reported as potential source of L-asparaginase. But reports from marine isolates are few.

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RECENT APPLICATIONS IN CAPILLARY ELECTROPHORESIS

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ABSTRACT: Capillary electrophoresis is an analytical technique that utilizes separation of ions based on their electrophoretic mobility with the usage of an applied voltage. The electrophoretic mobility is dependent upon the charge of the molecule, the viscosity, and the atom's radius. The rate at which the particle moves is directly proportional to the applied electric field - the greater the field strength, the faster the mobility. Neutral species are not affected, only ions move with the electric field. If two ions are the same size, the one with greater charge will move the fastest. For ions of the same charge, the smaller particle has less friction and overall faster migration rate. Capillary electrophoresis is used most predominately because it gives faster results and provides high resolution separation. Capillary electrophoresis (CE) is considered as a powerful method in many fields, such as biopharmaceuticals, environmental, food and public security analysis, owing to its high separation efficiency. However, the injection of small sample volumes and the short optical length lead to limited sensitivity. So it is necessary to couple with high sensitivity detector to realize the low concentration sample analysis. Capillary electrophoresis is a rapid and versatile electrophoretic technique that has found several applications. There are various applications of capillary electrophoresis like drug monitoring, single-cell analysis, diagnosis of metabolic disorders, sea water analysis, drug abuse. However, its greatest value for the characterization of synthetic peptides is when it is used in combination with other analytical techniques such as mass spectrometry, HPLC, and amino acid analysis.

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N-Directed Pd-Catalyzed Direct Ortho-Acetoxylation and Ortho-tert-butoxylation of 2-Phenyl-4H-Benzo[d][1,3]oxazin-4-ones via C-H Activation

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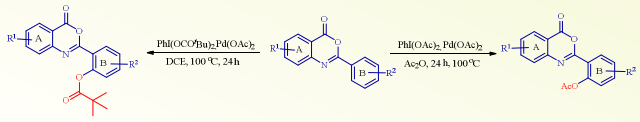
ABSTRACT: Last decade have witnessed the development of several straightforward strategies involving transition metal catalysts for the direct conversion of C-H bonds into C-X (X= C, N, O, S) bonds.[1] Among all of them, C-H oxygenations for the C-O bonds formation especially acetoxylationhas been identified as highly privileged approach .[2] Moreover, functional group assisted selective acetoxylation of inert C-H bonds of an aryl system has proven to be a highly diligent approach for the direct construction of C-O bonds.[3]

Taking an impetus from the enduring development of selective acetoxylation of C-H bonds and following our interest for the selective functionalization of valuable heterocyclic organic molecules,[4-5] we have achieved site-selective acyloxylation of 2-phenyl-4*H*-benzo[*d*][1,3]oxazin-4-one using [$PhI(OAc)_2$]/ [$PhI(OCO^tBu)_2$] as acyloxy source.



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IMMUNOMODULATORS: AN EMERGING THERAPY FOR ALZHEIMER'S DISEASE

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ABSTRACT: Alzheimer's disease is caused by the formation of amyloid beta plaques and neurofibrillary tau protein. There have been many therapies for treating Alzheimer's disease but immunomodulators are considered to be an emerging therapy for Alzheimer's disease. Immune system is now considered one of the important factor for Alzheimer's disease. There are different components of immune system such as central and peripheral immune system which plays an important part in Alzheimer's disease. In central there are different components that are involved in Alzheimer's disease, they are complement system, astrocytes and microglia; which are involved in Alzheimer's disease and in peripheral system components that are involved they are active and passive immunity further lymphocytes and neutrophilis that enters central system after the formation of amyloid plaques and tau protein. Immunomodulators may be the potential new players for treatment of Alzheimer's disease where direct therapies may failed to treat the disease. Many immunomodulators are under clinical trials to evaluate their effect in treatment of Alzheimer's disease.

KEYWORDS: Immunomodulators, Complement System

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Molecular basis of inhibitory action of Vitamin D on amyloid plaque, Tau, inflammatory and other signaling pathways mediating the progression of the Alzheimer's disease

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ABSTRACT: Background: Higher levels of Vitamin D are known to have a positive impact on cognitive impairment observed during Alzheimer's disease. Till now, Vitamin D has been highly researched for its probable strong association with key pathological factors of Alzheimer's disease due to wide distribution of vitamin D receptors across brain. Our preliminary*in-silico &in-vivo*study on Aβ1-42 model demonstrated neuroprotective action of Vitamin D and it improved cognitive function and decelerated progression of memory decline. AD prominently presents abundant formation of amyloid plaque,hyperphosphorylated Tau (p-Tau) and increase in inflammatory markers. Other than this, AD is also characterized by cholinergic deficits, synaptic loss and oxidative stress. Our aim was to investigate effect of Vitamin D on amyloid plaque (Aβ 1-42, Aβ 1-40), p-Tau and inflammatory markers such as TNF alpha, IL-6, IL-1β, NF-Kappa and to elucidate the effect of Vitamin D on other underlying downstream interconnected signaling pathways that are directly or indirectly associated with the induction or progression of the disease**.**

Methodology: Animals were grouped and subjected to neurobehavioral parameters testing. Alzheimer's disease induction was done usingScopolamine. Post induction, treatment was given as per the protocol & later animals were sacrificed for testing of biochemical parameters**Findings:** Long term administration of Vitamin D significantly improved cognitive function in Scopolamine induced Alzheimer's disease model in Wistar rats. Vitamin D altered all biochemical parameters which are known to play significant role in amyloid plaque, tau and inflammatory pathways. The results obtained are in consistent with our previous preliminary studies.

Determination of protein structure using Circular Dichroism

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ABSTRACT: Circular dichroism is most sensitive and widely used physical technique which is used in determination of structure and structural changes of biomolecules. Circular dichroism provides low resolution spectra but CD have two great strengths which makes is more of its use that are CD is extremely sensitive to conformational changes whatever their origin is, second with a small amount of material a wide range of solvent conditions are accessible. Circular dichroism is the differential absorption of left and right circularly polarized light by chiral molecules that is molecules that are non-superimposable on their mirror image form. Wide application CD is that estimation of β-protein, overlapping of various sheets bands and α-helix. CD uses light of U.V. radiation of far region that is lower wavelength.

CD is used in evaluating secondary structure, folding and binding properties conformation and stability and study of protein interaction . Various methods of estimating proteins structure using CD spectra involves ridge regression, singular value decomposition , variable selection, self constraint method.

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Implementation of Quality by Design : A Review

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Abstract: The term 'Quality by Design'(QbD) is an essential tool in the pharmaceutical environment to ensure that the quality of the product is free from any contamination,has assessed by performing in vivo and in vitro tests for evaluation.QbD plays an important role in development of todays growing pharmaceutical products. It provides guidance for designing ,development of molecules/products/formulations alsoprovide guidance for various manufacturing processes and analytical methods for pharmaceutical products.Accepting QbD as an important system in the pharmaceutical industries it has led to face many challenges to market their product. By using the QbD concept, regulators as well as industries are making a move to bring their products with better quality. Therefore, an attempt has been made to highlight quality by designing generic drugs and its implications to pharmaceutical industry including clinical trials, pharmaceutical validation processes and in biologics and also to provide a brief description on the status of QbD in India and as well as in Asia.

Phytochemicals with Neuroprotective Properties

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ABSTRACT: Currently, various neurodegenerative disorders, like Alzheimer's disease, depression, seizures, anxiety, cerebrovascularimpairment, Parkinson's disease, etc. are becoming predominant due to stressful lifestyle.

Long term treatment with synthetic drugs lead to various side effects. Therefore there is a need to explore the herbal drugs which can be usedfor treatment of neuroprotective disorders.

Various phytochemicals like alkaloids, steroids, terpenoids, saponins, phenolics, flavonoids, play a major role in maintaining the chemical balance of brain by actingupon the receptors of some important inhibitory neurotransmitters. Many medicinal plants like, *Bacopa monniera,Centellaasiatica, Celastruspaniculatus, Crocus sativus, Curcumalonga, Glycyrrhiza glabra,Salvia officinalis, Terminalia chebula, Uncariatomentosa, Valerianawallichii, Withaniasomniferaetc.*are being usedwidely in traditional system of medicinedue to their neuroprotectiveproperties.

Herbal antioxidants like polyphenols and flavonoids play neuroprotective roles by reducing or reversing cellular damage and by slowing progression of neuron loss.

Pomegranate juice improves behavior deficits and apple juice inhibits cognitive impairments. Several dietary flavonoids which are neuroprotecive in nature include epigallocatechin, epigallocatechin gallate, catechin, epicatechin, condensedtannins and proanthocyanidins.

Flavonoids like Apigenin and Luteolin which are found in artichoke, celery and parsley act as neuroprotective agents. Garlic and onion also have neuroprotective, properties due to presence of organosulfur compounds. Phytochemicals activate cellular stress-response pathwaysresulting in the upregulation of neuroprotective genes.

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A Recent update on WNT signalling modulators

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Abstract: Developmental signalling pathways control a vast array of biological processes during embryogenesis and in adult life. The WNT signalling pathway is an evolutionarily conserved signal transduction pathway that regulates a wide range of cellular functions during development including cell proliferation, cell fate determination, apoptosis, cell migration, cell polarity etc. during development and stem cell maintenance in adults. Recent advances have expanded the role of WNT to a wide range of pathologies in humans. This review collects different Wnt signalling modulators or inhibitors Since-2015 to till date. The molecules have been classified based on the role of WNT in different type of diseases, like Phase-I molecule of Novartis (LGKN974) acts via inhibiting porcupine for colorectal cancer; Phase-I molecule of ETC, Singapore (ETC-159) acts via inhibiting porcupine for advanced solid tumors.Samumed LLC, developedPhase-III moleculeLorecivivint (SM04690) acts via inhibiting WNT pathway for osteoarthritis of the knee. University of Madrid, Spain has developed ASS234 for Alzheimer's disease. CGX-1321 is in phase I clinical trials for advanced gastrointestinal cancers and RXC-004 is in phase I/II clinical trials for the treatment of solid tumors and many more. The role of Wnt in cancer development and its role in many other diseases has been confirmed by many studies. Therefore, the pharmaceutical discovery in both public and private institutions is still ongoing despite the plentiful molecules already published. However, many researchers are still looking for innovative Wnt modulation strategy for its role in different diseases.

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FORMULATION AND EVALUATION OF NANOCARRIERS BASED CYCLOSPORINE GEL FOR DERMATITIS

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Abstract: The objective of the study was to formulate microemulsion based topical drug delivery system for cyclosporine to improve transdermal permeation and aid to achieve site specific localized effect. The saturation solubility of drug was screened in various excipients from which Transcutol P was selected as surfactant, propylene glycol as co-surfactant and oleic acid as oil. Phase titration method was used to prepare microemulsion. Three ratios 1:1, 1:2, 2:1 of surfactant to co-surfactant mixture were selected for construction of pseudo ternary phase diagram. The 2:1 ratio showed maximum area in phase diagram and hence, it was taken for formulation of microemulsionof cyclosporine(20 mg/mL)and evaluated for particle size, zeta potential, pH, drug content, and *In-vitro* diffusion study. *In-vitro* diffusion study showed 100% drug release at the end of 6th hours. For the formulation of microemulsion based gel, Carbopol 943 was selected and different ratios were tried in which 1% and 2% showed better results.The *invivo* animal studies indicated no skin irritation with microemulsion based gelformulation. In dermatitis treatment, optimized gel formulation was found to be effective in both concentrations. Thereby microemulsion based transdermal drug delivery system can be explored for cyclosporine delivery in dermatitis.

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Development of Inosine-5'-monophosphate dehydrogenase (IMPDH) inhibitors against *Helicobacter pylori* infection.

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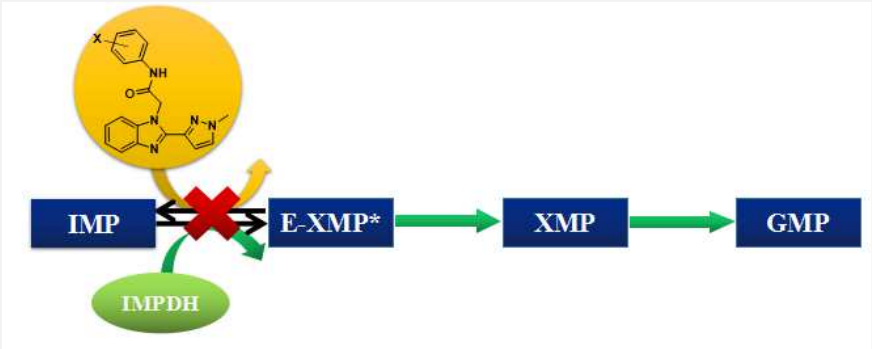
Abstract: *Helicobacter pylori*(*H.pylori*) is a Gram-negative, spiral-shaped bacterial pathogenassociated with human gastricmucosa, directly or indirectly causing peptic andduodenal ulcers, gastritis and gastric adenocarcinoma. Half of the world's populationis infectedwith*H. pylori* and the infection is much more in countries like India. Theability of thepathogen to survive in the highly acidic environment of stomach, andby virtue ofresistance developed by *H. pylori* strains, currently used antibiotic basedtreatments demonstrate high failure rates. Hence, there is an emerging need foridentification of new targets to treat *H. pylori* infection. Inosine 5' monophosphatedehydrogenase (IMPDH) is a crucial enzyme that catalyzes the rate-limiting step inthe *de novo* biosynthesis of guanine nucleotides. It converts IMP into XMP that isfurther converted into GMP which is required for the expansion of guanine nucleotide pool, responsible for cell proliferation. Thus, inhibition of *H.pylori* IMPDH presents potentialstrategy to treat *H.pylori* infection. Mizoribine, C91 and KJ73 are potent inhibitor andselective inhibitors of *Hp*IMPDH developed so far. Our work aims to overcome thedrawback of existing inhibitors by introducing refined benzimidazole scaffold fortargeting bacterial IMPDH. Here,we present our design, synthesis and *insilico*docking studies of benzimidazole scaffolds as *Hp*IMPDH inhibitors.



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Generic versus Branded Drug – Survey

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ABSTRACT: A generic drug is a chemically equivalent and a lower cost version a brand drug. A brand name drug and it's generic version must have same ingredient, dosage, safety, strength, usage direction, quality and performance. The cost can bereduce significantly from 30 to 80 % per prescription. When a company develops a new drug and submits it for approval a 20 year patent is granted. As the patent is near to it's expiry, any manufacturer can apply for it's generic version and it helps to reduce the cost. As these manufacturers don't have the same development cost,they can sell the drug at lower price.So to understand the use of generic drug in comparison of brand drug a survey was conducted among three category of populationi.e. Physicians -The one prescribing the medication ,People related to Pharmacy Sector and customers. A questionnaire was prepared for each group, data was collected from them, statistics were applied and inference was drawn based on result of the analysis.

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Silica Nanoparticles: A Revolution of Tomorrow

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Abstract: Nanoparticles are of paramount significance in the field of science as they form a fine bridge between bulk materials and atomic or molecular structures.The SiO_2 network can develop in a crystalline arrangement to form a material such as quartz or an amorphous arrangement in a material like glass.The amorphous form of silica can be synthesized as spheres on nano-meter scale through a base-catalysed sol gel process. . This synthesis method utilizes an organosilane precursor such as tetramethyorthosilicate (TMSO) or tetraethylorthosilicate (TEOS), represented as $Si(OR)_4$ where R is either a methyl (CH_3) or ethyl (C_2H_5) moiety- which undergoes hydrolysis and condensation.Silicon Nanoparticles can be defined as a system in which the diameter is in nano-scale i.e., Ranging below 100 nm. These are the preparation in which a drug compound can be loaded by various feasible means and are the current choice in R&D sectors as they hold a great potential to replace any kind of preparation which possibly shows a considerable amount in their properties.. The selection of appropriate method for the preparation of nanoparticles depends on the physicochemical character of the polymer and the drug to be loaded.MSN are used for targeted drug delivery at the target pH Triggered Release, Redox-potential Triggered Release, Enzyme Triggered Release. MSN have been investigated for the delivery of a variety of drugs including Non-Steroidal Anti-Inflammatory (NSAIDs) like Ibuprofen and Aspirin, antibiotics like vancomycin and chemotherapeutics such as doxorubicin and methotrexate.

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9. Sol–Gel Process and Applications in Controlled Release

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Design and synthesis of small molecule inhibitors targeting Tousled-like kinases (TLKs) as anti-cancer agent

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Abstract: Cancer is the second most global health problem. Overexpression or dysregulation of kinases is often in cancer. Therefore, protein/kinases are the major targets for the treatment of cancer. Targeting proteins/kinase involved in DDR (DNA damage response) pathway can have real therapeutic value in cancer therapy. Tousled gene was first identified in *Arabidopsis thaliana*, which are highly conserved in both plants and animals. It is a Serine/Threonine kinase. In mammals, there are two distinct TLK genes, TLK1 and TLK2, with several splice variants, have been recognized. They are involved in chromatin assembly and maintenance of replication fork integrity. Upon genotoxic stress, TLK1B is up-regulated and promotes DNA damage. The elevated expression of TLK1B was found in ~ 30% of breast cancer patients. Targeting TLK1/2, which is active S-phase and its relationship to these functions can result in effective and selective druggable targets for cancer therapy. *Ronald et al* identified the TLK inhibitors which belongs to the class of phenothiazine antipsychotics drugs using fluorescent high-through put screening. Thioridazine (THD) was found to be work specifically at low concentration. It is known to suppress the DNA damage response and improves therapeutic response in association with DNA damaging agents. The $–SCH_3$ group at position C2 in THD induces antipsychotic effect. Hence, our aim is to design the molecules which would better than THD and have a less antipsychotic effect. The use of newly synthesized and specific N-substituted fused heterocyclic-based inhibitors of TLKs could possibly identify the role of TLK mediated pathway and its significance in DNA damage and chromatin assembly.

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HOT MELT EXTRUSION : A PROCESS FOR SOLID DISPERSION

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Abstract: Hot Melt Extrusion (HME) is well known process for the Plastic Industries in 1930s but it is well accepted by the pharmaceutical industries for the last three decays. Solid dispersions represent a promising formulation approach for overcoming today's major challenge in pharmaceutical formulation development: poorly soluble and poorly permeable active APIs. Solid dispersions can be obtained using different processes; however, HME is extremely suitable for this purpose. One major advantage is the fact that no solvents are required. With the use of HME we can increase solubility and bio-availability of the API. Melt extrusion processes are currently applied in the pharmaceutical field for the manufacture of a variety of dosage forms and formulations such as granules, pellets, tablets, suppositories, implants, transdermal systems and ophthalmic inserts. HME has proven to be a robust method of producing numerous drug delivery systems like modified, sustained, controlled, targeted. HME has emerged as a powerful processing technology for the production of pharmaceutical solid dosage forms in which API is dispersed into polymeric matrices.

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Ultrasonic Studies Of Herbal oil With Some Cresols At Room Temperature With Fixed Frequency.

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Abstract : The binary mixtures of Herbal oil With Some Cresols containing different ultrasonic properties have been studied at room temperature at a fixed frequency of 2 MHz The ultrasonic related physical parameters like velocity (U), density (ρ), adiabatic compressibility (βad), intermolecular free length (Lf) ,acoustic impedance (Z).The result is interpreted in terms of molecular interaction such as dipole-dipole interaction through hydrogen bonding between components of mixtures. The dependence of excess properties of mixture compositions were compared and discuss in terms of the intermolecular free length and other factors affecting the salvation and self association effect. The excess values of these indicate dipole-induced dipole interaction complexity in the binary liquid mixture

Key words - ultrasonic velocities, thermodynamic parameters, acoustic impedance, intermolecular free length

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Evaluation of Anti-cancer and Anti-invasion activity of Curcumin Multicomponent Solids against 2D Monolayer Culture and 3D Tumor Model of a Triple Negative Breast Cancer (TNBC) Cell line

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Abstract: Curcumin (CUR) is a natural polyphenolic compound present in the rhizome of Indian spice, turmeric (called as *Curcuma longa*). However, its bioavailability is limited due to its low aqueous solubility and it has been classified by Biopharmaceutics Classification System (BCS) under BCS class IV category (Tonnesen, 2002). In this work, we report the anti-cancer and anti-invasion activity imparted by CUR solid phases (cocrystals/eutectics/coamorphous solid) prepared by various cocrystallization techniques such as Eutectic melt cum Evaporative Crystallization (EC), Liquid-Assisted Grinding (LAG) and Solid-State Grinding (SSG) on 2D monolayer and 3D spheroid cultures of a Triple Negative Breast Cancer (TNBC) cell line, MDA-MB-231. These CUR solid phases includes curcumin-hydroxyquinol (CUR-HXQ) (1:1) cocrystal (Sathisaran and Dalvi, 2017), curcumin-folic acid dihydrate (CUR-FAD) coamorphous solid (1:1) (Skieneh et al., 2017), curcumin-salicylic acid (CUR-SAA) (1:2) eutectic (Sathisaran and Dalvi, 2017), curcumin-paracetamol (CUR-PAR) (1:3) eutectic and curcumin-succinic acid (CUR-SUC) (1:1) eutectic (Sathisaran et al., 2018). Curcumin was found to possess Minimum Inhibitory Concentration (MIC) of 10 µM. Cytotoxicity assay and cellular uptake assay in 2D monolayers followed by Cell invasion assay in 3D spheroids prepared by Hanging Drop Culture method (Shri et al., 2017) were conducted with CUR solid phases containing 10 µM of CUR concentration. Cytotoxicity assay conducted in 2D monolayers for 24 hours with 10 µM CUR revealed that CUR-HXQ (1:1) cocrystal showed enhanced cytotoxicity than the rest of the solid forms while CUR-FAD (1:1) coamorphous solid showed growth effect in the cells than the raw CUR. Also, the CUR uptake for 24 hours was found to be maximum with MDA-MB-231 cells treated with CUR-HXQ (1:1) than the other solid forms. Surprisingly, from the cell invasion assay carried out in the 3D spheroid model we observed that CUR-HXQ (1:1) cocrystal arrests the cell migration efficiently whereas CUR-FAD (1:1) coamorphous solid facilitated cell migration. Therefore, we propose that though combinatorial drug therapy via cocrystal engineering is an effective approach for anti-cancer treatment, the choice of coformers affects the efficacy of CUR. CUR-HXQ (1:1) cocrystal possess an effective anti-breast cancer activity possess an effective anti-breast cancer activity whereas CUR-FAD (1:1) coamorphous solid is proposed to be not suitable for cancer therapy.

Keywords: Curcumin, cocrystals, eutectics, co-amorphous solid, CUR-HXQ (1:1) cocrystal, CUR-FAD (1:1) coamorphous solid, cell invasion, anti-breast cancer

Figure 1. CUR uptake by MDA-MB-231 cells treated with (A) CUR-HXQ (1:1) cocrystal, (B) CUR-FAD (1:1) coamorphous solid, Cell invasion arrest in MDA-MB-231 3D Spheroid model treated with (C) CUR-HXQ (1:1) cocrystal and (D) CUR-FAD (1:1) coamorphous solid

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Marketing Authorization Requirements for African Countries and Comparison with USA Market

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Abstract : As the market for the pharmaceutical industry is rapidly growing that is because of advancements in technology related to the formulation. It has been seen that as such there is an increase in the market authorization given by specific nation regulatory authority. Likewise, there is a market authorization for African countries where the documents need to be compiled and submit in CTD format only. As the countries of such continent have not been so much stringent as the US or EU. There are many cases where the difference in prior submission to final approval can be seen. Though these countries are developing countries it has been seen that there are guidelines that need to be followed for registration of medicines for those specific nations. For generics, there are not many specific requirements which can be varied as from that novel drugs. The fees, document filing, approval, validity, label requirements are some of the differences to note down for registration. The US market is more reliable as compared to African nations. The final approval decision relies on regulatory authority. e-CTD is mainly the requirements for the US market. The DMF is the general requirement for any country.

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New age antimicrobial peptides: Revealing mode of actions of multifunctional AMPs using modelcular dynamics study

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Abstract: Currently, antimicrobial resistance developed by many infectious pathogens is a severe emerging problem. Antimicrobial peptides can be used as potential alternatives to conventional antibiotics because of their multi functionality and non-specificity in targeting pathogens. To understand different mechanisms of killing via bacterial membrane by AMPs in detail and to see differences in the mode of action of two peptides, Magainin2 and Pleurocidin with different modes of action we performed Molecular Dynamics simulations. Experimentally, Magainin2 is known to form toroidal pores in the membrane whereas Pleurocidin is known to interact with the intracellular targets. Molecular dynamic simulations were run for both peptides and for each orientation for 100-1000 ns using Gromacs and the charmm36m force field. Modelling a bacterial membrane (POPE:POPG in 3:1) solvated in the TIP3P water model and 0.15M NaCl ions.

Magainin2 was found to significantly disrupt the membrane by forming toroidal pores, however Pleurocidin also seemed to be form pores when forced in the membrane.

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Design development and evaluation of cationic lipid conjugated nanostructured lipid carrier with a natural terpenoid.

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Abstract: The aim of the present study is the evaluation of cationic lipid conjugated natural terpenoid for brain targeting and neurological disorders. Natural bioactives are very potent and lots of mechanisms to improved the neurological disorders but due to their hydrophobicity and short biological half life, these are not able to reach at the targeted site. In lieu of this the nano approaches are developing to overcome these hurdles. Now, nanostructure lipid carrier (NLC) is a new tool for targeting the drug into the brain and better management of various neurological disorders. Here, cationic lipid conjugated NLC was prepared with a natural terpenoid with QBD designs. Various characterization studies were performed. *In -vitro* release studies were performed of the formulation with drug solution with different kinetics models. Cell line studies were done with SH-SY-5Y neuroblastoma cell lines. Various *in- vitro* evaluation studies like MTT assay, cellular uptake studies were done for different time points. Finally it is concluded that the cationic lipid conjugated NLC provided more effectively than the drug solution and normal NLC. In future pharmacokinetic and pharmacodynamic studies with animal model will be performed.

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FORMULATION DEVELOPMENT OF SUBLINGUAL TABLET FOR MIGRAINE TREATMENT

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Abstract: Migraine is a very common neurobiological headache disorder that is caused by increased excitability of the CNS and excessive vasodilation.Sumatriptan, Rizatriptan, Naratriptan, Amlotriptan, eletriptan, frovatriptanare recommended as first-line drugs for patients with moderate-to-severe migraine. Conventional oral delivery has comparatively slow onset of action about,due to slower absorption from gastric mucosa and having oral bioavailability 65% to 70% due to gastric and intestinal absorption. Moreover, oral delivery exhibits side effects like burning type of sensation, which leads to patient incompliance [1]. Sublingual route may overcome abovementioned issues, by releasing the drug in to oral cavity and promotes major absorptions from oral mucosa. Low dose, low molecular weight and good permeability ofthe drug makes it suitable candidate for sublingual delivery [2]. The aim of the present research work was to develop rapidly disintegrating sublingual tablet. In this study various disintegrating agents and diluents were explore such as sodium starch glycolate, Crosscarmellose sodium, Cross PVP and Polacrillin Potassium(Kyron T-314) as superdisintregrating agents Mannitol, Microcrystalline Cellulose, lactose anhydrous as diluents.Preformulation studies such as angle of repose, Bulk density, Tap density were perfomed.The tablets were prepared by direct compression and evaluation was done by performing various tests such as weight variationtest, friability, thickness, hardness, disintegration time and wetting time [3]. It was observed that concentration of diluents and disintegrating agents has significant effect on the disintegration time of tablet formulation. Approach of formulation of sublingual tablet of will increase onset of action and reduce side effects as mention above.

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DEPRESSION RELATED TO PCOS; A THIEF OF WOMANHOOD

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Abstract: Polycystic Ovarian Syndrome (PCOS) is an endocrinopathy of reproductive age women andits incidence is increasing due to change in lifestyle and stress. Women with PCOS are at an increased risk for primary and secondary infertility, pre-eclampsia, early pregnancy loss andendometrial cancer. (Nanjaiah & Roopdevi,2018).The increased prevalence of PCOS amonggeneral population throughout the world is found to be 5% -10% in the women of reproductiveage, and about 40% women with PCOS experience depression. (Sadeeqaetal,2018).It is thecommon illness that severely limits the psychosocial functioning and diminishes quality of life.In 2008, WHO ranked major depression as the third cause of burden of diseaseworldwide and projected that the disease will be rank first by 2030. (Malhi & Mann, 2018). Pathophysiologyof PCOS is still unclear, although there is evidence that both genetic and environmental factorscan play role resulting in ovarian hyperandrogenism. The symptoms include amenorrhea,hirsutism, infertility, obesity, acne vulgaris and andandrogenic alopecia. PCOS is astigmatizing condition that affects woman's identity, mental health and Quality of Life (QOL).This aspect has not received adequate attention in India. (P. Chaudhari etal, 2018). There aresome common points of association between PCOS and Depression like hypercortisolaemia,levels neurotransmitter (low in both the cases), elevated MAO levels. Hence, we can proposethe question for future research that antidepressants can be the potential targets for PCOS andvice versa

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Development of nanostructured lipid carriers of Resveratrol for nose to brain targeting

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ABSTRACT: Nanotechnology based treatment, especially for diseases where targeting is required, is now being used in developing countries. The objective of present research work was to also to investigate the targeting of resveratrol in brain using nanostructured lipid carriers (NLCs) and incorporate the NLCin in-situ gel to facilitate administration via nasal route, followed by evaluation in animal models for treatment of alzheimer's disease.Oral administration of resveratrol shows poor bioavailability (only 40%) due to extensive first pass metabolism, which can be avoided by nasal administration of the drug. The NLCs of resveratrol were prepared by melt emulsification - probe sonication method.The screening of important factors governing performance of the NLCs were done using thePlackett Burman design. The optimization was done using2^3full factorial design where drug concentration (X_1: 5-10 mg), surfactant concentration (X_2: 50-350 mg), solubilizer concentration (X_3: 100-200 mg) were selected as independent variables. The NLCs were prepared, characterized and dispersed in gellan gum and xanthan gum solution to prepare in-situ gels. The particle size, zeta potential, PDI, drug loading, entrapment efficiency of optimized batch was 118 nm, -21 mv, 0.413, 17 % and 88 % respectively. The optimized batch showed clear appearance, pH- 6, excellent gelling capacity, CIC- 0.2 ml, expansion coefficient- 1.02 %, viscosity- 234 and 4865 cps before and after gelation respectively, gel strength - 48 seconds and 73.76 % permeation across sheep nasal mucosa as compared to pure drug containing in-situ gel. Resveratrol NLCs based in-situ gel showed better performance in term of drug concentration in brain compared to conventional suspension. In conclusion NLC based in situ gel can be a promising targeting system for CNS diseases.

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Multi-target Binding Profile of Tetrahydrocannabinol: Conformational Variations Analysis

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Abstract: Tetrahydrocannabinol (Δ^9THC) is a psychoactive chemical obtained from Cannabis sativa plant. It is extensively abused throughout the world mostly through illegal use. THC alters the perception creating an altered feeling. Mammalian brain is known to possess specific receptors for THC like natural molecules present in the body. Though THC is a banned drug, its therapeutic potential is being actively investigated. It is known that THC has beneficial effects in epileptic patients in controlling the seizures, affect cognitive capacity and in some cases enhances the focus/concentration. Due to its apparent health effects, it is essential to investigate the possible biological targets in the living system. The present study demonstrates that THC binds with DNA and other protein receptors with moderate affinity. DNA binding results show that its binding in the minor groove is accompanied by a significant conformational alterations.

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Evaluation of Some New Heterocyclic Compounds as Potent Antibacterial Agents against Human Pathogens

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Abstract: Tetralone scaffold have been a part of major fundamental classes of compounds showing distinct biological activities such as antibacterial, anticancer, antifungal, COX-2 inhibitors, anticonvulsant, anti-parkinson as well as antidepressants whereas quinoline synthetic derivatives have also shown antibacterial, antifungal, antimalarial, antimycobacterial, anticonvulsant, anti-inflammatory, cardiovascular and anticancer activities. In our study, several heterocyclic compounds having tetralone and quinoline scaffolds were synthesized and evaluated for their antibacterial activity against both Gram positive and Gram negative bacterial strains. The *in vitro* antibacterial activity was analyzed by 96 well plate microdilution method. The potent compounds among the tetralones were found to inhibit the growth of wide range of bacterial strains *Salmonella typhi* (MTCC 733), *Enterobacter aerogenes* (MCC 3092), *Klebsiella pneumoniae* (MCC 3094), *Pseudomonas aeruginosa* (MCC 3097), *Shigella flexneri* (MCC 3095), *Serratia marcescens*, *Staphylococcus aureus* and *Bacillus subtilis* while potent compounds among quinoline were found to inhibit the growth of *Enterobacter aerogenes* (MCC 3092), *Pseudomonas aeruginosa* (MCC 3097), *Shigella flexneri* (MCC3095), and *Escherichia coli* (MTCC 1610). The results showed that the tetralone and quinoline derivatives used in our study are potent new antibacterial molecules against human pathogens.

Keywords: Tetralone, Quinoline, Antibacterial activity, Human pathogens, Microdilution

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Isolation & Identification of Chemical Constituents from *MenthaSpicata*Leaves

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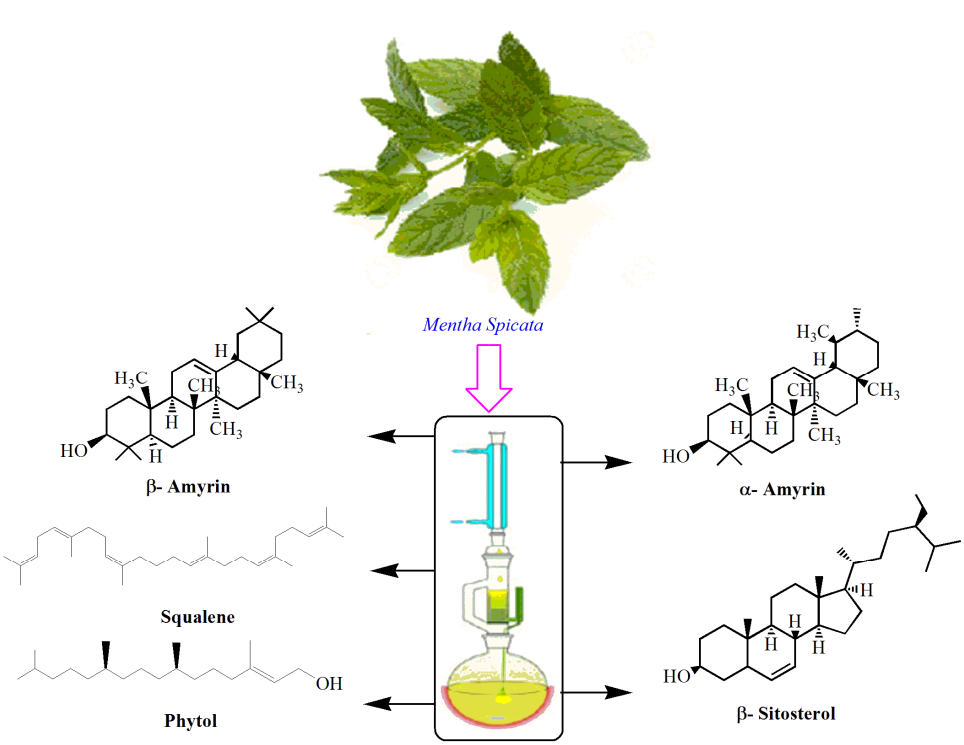
Abstract: Investigations were carried out to isolate and determine the chemical constituents of *Menthaspicata*leaves, a medicinal plant used in folklore. The leaves were extracted with petroleum ether for this study. After saponification process fatty acid was separated and extraction was carried out using diethyl ether. Using gradient elution in column chromatography three compounds were identified and one compound was isolated. All the fragments were identified by GC-MS hyphenated technique and one isolated compound was analysed by ^{1}H NMR, ^{13}CNMR and elemental analysis. From this study concluded that Squalene, Phytol, Amyrin were identified and beta- Sitosterol was isolated from the leaves of *Menthaspicata.*



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E-Pharmacies in India

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Abstract: Buying drugs/medicines online is the latest trend amongst the Indian patients and consumers. With this increasing trend of buying medicines online, number of online pharmacies also increase. But there is lack of proper regulatory checks and balances for exercising regulatory control over e-pharmacies. There are several other factors also which fuel the gearing up of e-pharmacies like increased number of netizens, long term illness patients and increased chronic diseases. As we all know India is the country of youngsters and they are spending more and more time on internet through mobile or computer. Due to the advancement of technology, access of drugs through Internet is very easy for common man. This is the high time for the e-pharmacy model to grow with the drastically increasing netizens, smart phone users and patients. E-pharmacies business is growing very fast in India although its mechanism of regulation is not decided yet. There is lack of proper and clear laws for e-pharmacies. The laws governing Pharmacies in India are derived from Drugs and Cosmetics Act, 1940; Drugs and Cosmetics Rules, 1945; Pharmacy Act, 1948; Indian Medical Act, 1956 and Code of Ethics Regulations, 2002 etc. E-pharmacies come under the purview of the Drugs and Cosmetics Act, 1940 and the Information Technology Act, 2000. But current Drugs and Cosmetics Act, 1940 doesn't distinguish between online and offline pharmacies. It seems e-pharmacies may not abide by these regulations and bypass them. Regulatory authorities finds it difficult to control, monitor and track sell of drugs via internet as there is lack of clear guidelines in India regarding the same. E-pharmacy may be proved as dangerous trend in future if not regulated properly.

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Anti-HIV treatment: Recent Updates

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Abstract: Human Immunodeficiency Syndrome (HIV) virus acts as an etiologic factor for the occurrence of Acquired Immunodeficiency Syndrome (AIDS).Over 35 million people are infected with HIV-1.According to statistics provided by WHO reports, 1.8 million people were additionally infected by HIV and 1 million people were reported to be dead because of HIV in 2018. Because of the availability of HAART therapy HIV associated deaths have decreased by 39% since 2000 (Tian Ye et al).An important target for the action of anti-HIV therapy is the Reverse Tanscriptase enzyme. Currently, there are two types of Reverse Transcriptase enzymes (RT) currently available- Nucleoside Reverse Transcriptase Inhibitors (NRTIs) and Non- Nucleoside Reverse Transcriptase Inhibitors(NNRTIs). Out these, NNRTIs have a non-competitive action on RT and are an important part of Highly Active Antiviral therapies(HAART).In the late 20th century, Efavirenz and Nevirapine were approved but after more than 2 decades of continuous therapeutic use, NNRTI resistant mutants emerged.To tackle with the problems of emerging resistance,NNRTIs of the second generation like Etravirine and Rilpivirine were discovered. Most of these compounds contain diarylpyrimidine nucleus and show a higher genetic barrier to already mutated viruses as they have the ability to change their conformation and owing to this flexibility they can bind in different conformations to the Reverse Transcriptase.However, resistance to the agents like Tenofovir/ Emtricitabine/ Rilpivirine also emerged and these mutations were resistant to NNRTIs and NRTIs.

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Liposome as a carrier foranticancer drug

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Abstract: Cancer is a life-threatening disease contributing about 3 to 4 million deaths worldwide. The first-line treatment of cancer is the surgical removal of solid tumors, radiation therapy, and chemotherapy. Cancer leads to irregular and uncontainable growth of malignant cells.There are different approaches to treat cancer but among all of that lipsome are best to treat cancer.Liposome based drug delivery systems offer the potential to enhance the therapeutic index of anti-cancer agents, either by increasing the drug concentration in tumor cells and/or by decreasing the exposure in normal tissues exploiting enhanced permeability and retention effect phenomenon and by utilizing targeting strategies. The success of cancer treatment basically depends on its capability to decrease the size and remove tumors without affecting normal tissues.A liposome is a spherical vesicle having at least one lipid bilayerandmade up of the same material as a cell membrane. Liposomes can be filled with drugs, and used to deliver drugs for cancer and other diseases. Liposome mainly contains cholesterol and phospholipids. Liposomes have a hydrophilic head group and a hydrophobic tail group. Liposome can carry both hydrophobic molecules and hydrophilic molecules. Liposomes characterize an advanced technology to deliver active molecules to the site of action. The site avoidance and site-specific drug targeting therapy could be achieved by formulating a liposomal product. Problem with liposome is that it may not reach to the site of action due to RES(Reticulo endothelial cell) which is recognize as a foreign material so these are destroyed by RES. To overcome this problem surface modification can be done.To protect it from the gastrointestinal environment, coat liposomal surfaces with layers of polymers such as enteric polymers, protein. Enteric coatings are well known to prevent liposomes from disintegration in the stomach thereby improving absorption as more liposomes survive and are exposed in small intestine. There isalso an another approach to coat with such receptors so it can easily reach tothe target and not destroyed by the RES.Folate coated liposomes reach at the site where it can bind and act on tumor. Liposome is having disadvantage like leaking of drug which is a major challenge and can be overcome by various approaches.

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Nanosilver as a new generation nanoproduct and it's applications in wound healing.

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Abstract: Nanosilver (NS), comprising silver nanoparticles, is attracting interest for a range of biomedical applications owing to its potent antibacterial activity. It has recently been demonstrated that NS has useful anti-inflammatory effects and improves wound healing, which could be exploited in developing better dressings for wounds and burns. The key to its broad-acting and potent antibacterial activity is the multifaceted mechanism by which NS acts on microbes. This is utilized in antibacterial coatings on medical devices to reduce nosocomial infection rates. Many new synthesis methods have emerged and are being evaluated for NS production for medical applications. NS toxicity is also critically discussed to reflect on potential concerns before widespread application in the medical field.

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Insights into Therapeutic Perspectives of Prion's Disease

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Abstract: Prion disease (PrDs) are a group of neurodegenerative disorders caused by infectious protein called prions protein. Prion diseases or Transmissible Spongiform Encephalopathies, are fatal neurodegenerative conditions that affect humans and other animals, and are transmissible within or between mammalian species by inoculation or ingestion. Human PrDs occur in three ways: sporadic (spontaneous), genetic, and acquired. This disease was first identified in the 1732 in the sheep. There is no current medication available for the disease. The Prion Protein PrP exists in two major isoforms: the non-pathogenic or cellular form (PrPC) and the pathogenic or scrapie-inducing form (PrPSC). The formation of PrPSc is favoured by the presence of a mutation of PRNP that destabilises the mutated native PrNP. The methionine (M) to valine (V) polymorphism at codon 129 of PRNP could a□ect the disease phenotype and some of the characteristics of the disease-associated PrPSc. We will also be discussing about the recent updates about the disease.

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Formulation and Characterization of Meloxicam Loaded Nanostructured Lipid Carriers (NLCs) for Treatment of Arthritis

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Abstract: The main objective of the study was to formulate and characterize Meloxicam loaded Nanostructured lipid carriers (NLCs) incorporated gel to achieve its enhanced permeability and controlled release. Meloxicam is a non-steroidal anti-inflammatory drug (NSAID) that is used for the treatment of arthritis as it reduces the inflammation and provides symptomatic relief. Topical delivery of meloxicam loaded NLCs incorporated gel can be beneficial to surmount the oral side effects and achieve controlled therapy and enhanced permeation. The selection of solid lipid and liquid lipid for the formulation of meloxicam loaded NLCs was done on the basis of the solubility of meloxicam in various lipids. The highest solubility of meloxicam was observed in compritol HD5 ATO and oleic acid thus they were selected as solid lipid and liquid lipid respectively for the formulation of NLCs. Amongst various surfactants, tween 80 was selected as it represented minimum solubility of meloxicam in it and imparted good stability to NLCs. The method of preparation employed was hot melt homogenization technique and effect of various factors like effect of surfactant type, surfactant concentration, homogenization speed and homogenization time on NLCs characteristics were evaluated. They were characterized for particle size, zeta potential, polydispersity index(PDI), entrapment efficiency, differential scanning calorimetry(DSC), transmission electron microscopy(TEM) and in-vitro drug release. Carbopol 937(1%) was selected as a gelling agent on the basis of its rheological properties, pH, highest liquid uptake, spreadability and stability. The formulated nanoparticles had desired particle size, sphericity, morphological characteristics, entrapment efficiency and in-vitro release profile.

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ROSTRAL MIGRATORY PATHWAY

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Abstract: Rostral migratory stream is the pathway by which the drug can be directly administered to the brain. It consists of mainly olfactory bulb and sub-ventricular zone, which extends to the various parts of the brain. Conventional methods such as intraparenchymal routes, intraventricular route or by increasing the dose, can lead to toxicity and can even cause patient incompliance.Rostral migratory stream can be even used to deliver the stem cells to the brain which can help in the neuronal regeneration. This will lead to the cure towards neurodegenerative disorders like alzhiemer's disease and Parkinson disease without the unwanted toxic effects. Moreover, drugs administered by this route reaches the C_{max} very rapidly in the brain so the drugs which are poorly permeable to the BBB (Blood Brain Barrier) can also be administered by this route. As the drug is also directly administered to the brain, it is has rapid onset of action with negligible peripheral adverse events.

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RECENT THERAPEUTIC TARGETS IN ALZHEIMER'S DISEASE:

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Abstract: Alzheimer's is a wide spread neurodegenerative disorder in the world which causes dementia in people. The main epidemiology and the most people affected by this disease are the old age people. Alzheimer's disease is mainly caused by the genetic factors, age, improper cleavage of amyloid β and τ proteins leading to neurodegenration. The disease is very much vulnerable and there are currently only 5 drugs available which is approved US-FDA. In this poster presentation, we will be discussing about the various targets of alzheimer's like targeting β-amyloid, τ-protein targeting, caspase inhibitors, microglia targeting, micro-RNA targeting.

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Pharmacophore Modeling, Virtual Screening, Docking and *In Silico* Toxicity Prediction Studies of *Human* Dihydroorotate Dehydrogenase (*h*DHODH) Inhibitors

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Abstract: Fourth step in *de novo* pyrimidine biosynthesis is oxidation of dihydroorotate (DHO) to orotate (ORO) catalysed by rate limiting enzyme dihydroorotate dehydrogenase (DHODH). Pyrimidine bases are required for biosynthesis of DNA, RNA, glycoproteins and phospholipids and essential for the cellular metabolism and cell growth. *Human* Dihydroorotate Dehydrogenase (*h*DHODH) is a recognised target for the development of new drug candidates against cancer, rheumatoid arthritis and multiple sclerosis. Herein, we describe pharmacophore-modeling and virtual screening combined with docking study as a rational strategy for identification of novel hits or leads as *h*DHODH inhibitors. A total number of 12 known *h*DHODH inhibitors were used to generate pharmacophore models applying DISCOtech and GASP. Virtual screening was performed to search IBS database. A total of 34 compounds were identified as good *h*DHODH inhibitors. Among these molecules, those who have a Qfit value more than 90% were docked on *h*DHODH to further explore the binding mode of these compounds. Finally *In silico* toxicities were predicted for best docked molecules. The hits reported here showed good potential to be *h*DHODH inhibitors.

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P-228

ANTIOXIDANTS, FLAVOUR ENHANCERS AND STABILZERS USED IN THE FOOD PRODUCTS

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Abstract: Food additives are substances that food manufacturers intentionally add to food in small quantity during production or processing to improve the organoleptic quality (colour, flavour, appearance, taste and texture) of the food. They help to increase the shelf life of the food by maintaining product consistency and freshness; also added to food to preserve flavour or enhance its taste and appearance. In the second half of the 20th century, many more additives have been introduced, of both natural and artificial origin. As all food components, they are classified based on their function in the food products. We will be discussing various natural and synthetic substances which are used as additives (antioxidants, flavour enhancers and stabilizers) in the food product and also the analytical techniques used for identification of such substances. We will also be discussing the Guidelines for antioxidants, flavour enhancers and stabilizers.

P-229

A Study of Neurological Activity from Tabernaemontana Divaricata Plant

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Abstract: Neurodegenerative diseases are the brain disorders with selective loss of neuronal activity, degeneration of neuronal cells and distinct involvement of the functional movements. The major Neurodegenerative Disorder that affects memory, cognition & Behavioural Impairment (Mood Fluctuation & Fatal Delirium). The specific pathologies lies in Alzheimer's disease includes Amyloid β Protein Hypothesis, Tau Polymerase, Mitochondrial Cascade Hypothesis and Acetylcholinesterase. In Current scenario now there are 5 FDA approved drugs that worked on cholinesterase inhibitors and NMDA antagonist. Neuroprotective Agents refers to substances that are capable of preventing Brain Function and Structure By reducing and preventing Oxidation Stress, Mitochondrial dysfunction, Inflammation, various forms of Neurotoxicity (E.g.) Excitotoxicity and Protein deficiencies.Beside continues used of Allopathy medicines which interact with multiple brain function, result into addiction of drug causes various side effects. Tabernaemontana Divaricata (F: Apocynaceae) have been used in curing various disease such as eye, skin, dental disease and also used in Thai medicine as Neurotonic and analgesia. This review will help in cumulative study of plant in Alzheimer's disease.

P-230

Design, synthesis and antimicrobial activity of novel 1,3,4-oxadiazoles incorporating pyrazole scaffolds

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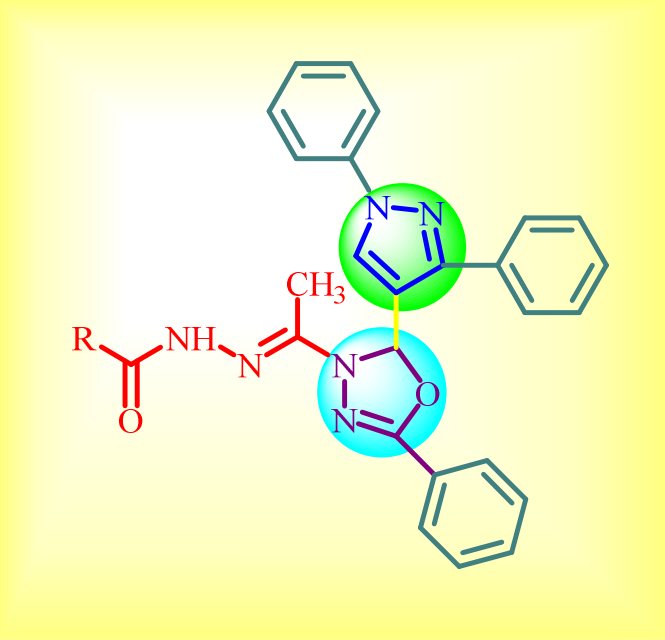
Abstract: In search of new antimicrobial agents with improve potency, we have synthesized *N'*-(1-(2-(1,3-diphenyl-1-*H*-pyrazole-4-yl)-5-phenyl-1,3,4-oxadiazole-3(2*H*)-yl)ethylidene)-(aryl)-benzohydrazidesby combining 1,3,4-oxadiazole and pyrazole scaffolds having diverse pharmacological activities. All the newly synthesized compounds werecharacterized by different analytical techniques like IR, ^{1}H and ^{13}C NMR and mass spectrometry. These compounds have been evaluated for their *in vitro* antimicrobial activity against Gram-positive bacteria *Staphylococcus aureus* (MTCC 96), *Streptococcus pyogenes* (MTCC 442), Gram-negative bacteria *Escherichia coli*(MTCC 443),*Pseudomonas aeruginosa* (MTCC 1688), fungi *Candida albicans* (MTCC 227), *Aspergillusniger* (MTCC 282) and *Aspergillusclavatus* (MTCC 1323) using serial broth dilution method. From the results, it was found that compounds with electron withdrawing groups showed excellent antibacterial activity while compounds with electron donating group showed very good antifungal activity.



P-231

Association of Vitamin D deficiency and mood disorders: A Systematic Review

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Abstract: The cells of our body comprise of calcitriol (1, 25(OH)vitamin D_2), the active form of vitamin D, an integral biological substance that has an impact on a large number of biological processes. While high prevalence of Vitamin D deficiency is detected in population worldwide, the reports from sun-soaked countries like India are also alarming to note that, the deficiency of Vitamin D as high as 70 to 90% is observed leading to several chronic diseases in the majority of people. Deficiency of Vitamin D is observed not only because of low levels of vitamin D in diet, less exposure to sunlight, reduced cutaneous vitamin D synthesis, but also due to consumption of particular medicines, undue alcohol intake, and tobacco smoking. Vitamin D is known to affect estradiol, dopamine, pro-inflammatory cytokine levels, besides involved in the regulation of mechanisms pertaining to hormones like glucocorticoids. When vitamin D binds to Vitamin D Receptors present in central nervous system, it is noted to be responsible for regulation of brain-neuronal functions. Low 25- hydroxy Vitamin D levels are found to have the higher incidence of various mood disorders. This review focusses on vitamin D receptors, VDR gene mutations and pathophysiology causing vitamin D deficiency disorders.

P-232

Synthesis and characterizationof some 1, 3, 4-oxadiazole-furan hybrids as antitubercularand antibacterial agents

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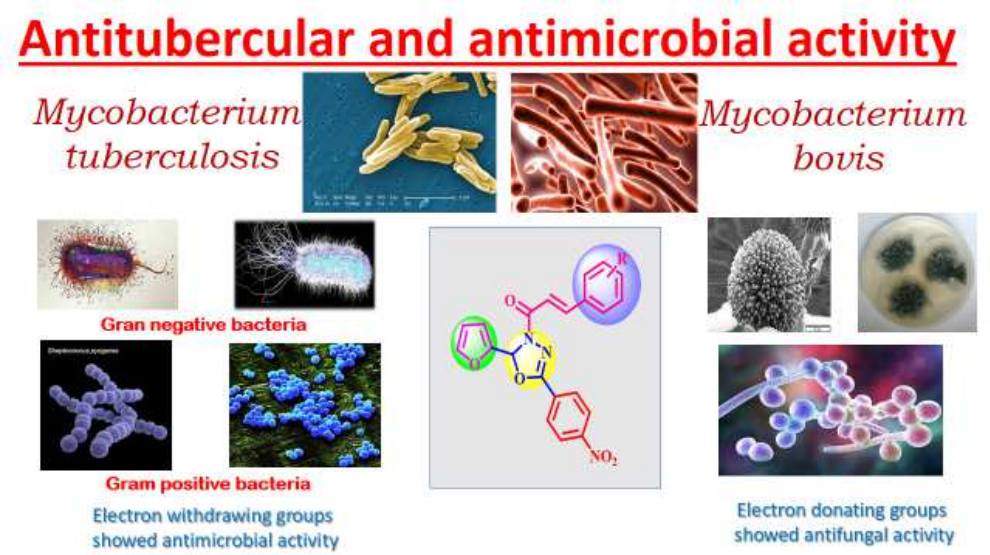
Abstract: A series of 1-(2-(furan-2-yl)-5-phenyl-1,3,4-oxadiazol-3(2*H*)-yl)-3-(aryl)prop-2-en-1-oneswere obtain by combining 1,3,4-oxadiazole and pyrazole scaffolds. Structures of all the newly synthesized compounds were confirmed using different analytical techniques like IR, ^{1}H and ^{13}C NMR and Mass spectrometry. These compounds were evaluated for their *in vitro* antimicrobial activity against Gram-positive bacteria *Streptococcus pyogenes* (MTCC 442), *Staphylococcus aureus* (MTCC 96), Gram-negative bacteria *Pseudomonas aeruginosa* (MTCC 1688), *Escherichia coli* (MTCC 443),fungi *Aspergillusniger* (MTCC 282), *Candida albicans* (MTCC 227) and *Aspergillusclavatus* (MTCC 1323) using serial broth dilution method. It was found that compounds with electron withdrawing groups showed excellent antibacterial activity while compounds with electron donating group showed very good antifungal activity. The synthesized compounds were further screened for antitubercular activity against *Mycobacterium tuberculosis*H_{37}Ra (ATCC 25177) and *M.bovis* (ATCC 35734) strains using rifampicin as a standard antitubercular agent. The synthesized compounds were found to possess promisingantitubercular activity.



P-233

Extraction of active ingredients from aerial parts of solanum xanthocarpum (Sol.xan)

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Abstract: Plant species *solanum xanthocarpum(Sol.xan)* is selected forpresent study of phytochemical properties like anti-oxidants, antimicrobial,sterols and flavonoids. This plant has high medicinal property like anti-fertility activity, anti-hyperlipidemic activity, hepatoprotectiveactivity, antimicrobial activities etc. *Sol.Xan* species contain various chemical constitution Solasodine,Esculetin,Caffeic acid,Oleanolic acid. The plant samples were collected in seasons of monsoon and arability of this plant in rural area of Bhavnagar. Different parts of plant were isolated and oven dried at 60ºC for 48hours. Extraction of crude material from aerial parts of the plants were carried out by the soxhlet extractor and four different solvents *viz*. water, ethyl acetate, 1,2 dichloroethane and n-hexane to extract the various groups of phytochemicals. The crude is further subjected to TLC for confirming the extraction of various ingredients of our interest, which can be further utilized for screening of antimicrobial activities.

P-234

Hybrid heterocyclic compounds bearing pyridine and oxadiazole scaffolds as potential antimicrobial agents

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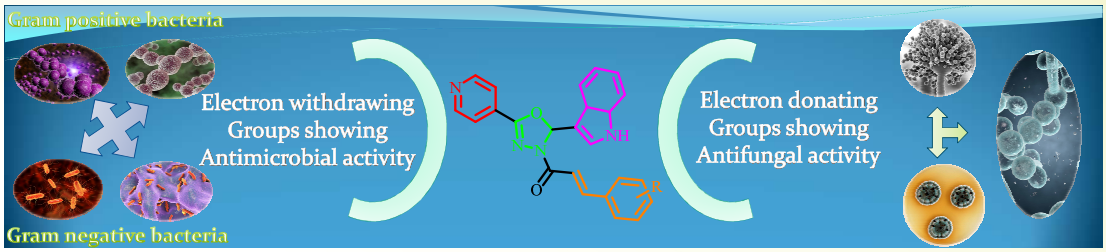
Abstract: 1,3,4-oxadiazole heterocycles are very good bioisosteres of amides and esters, which can contribute substantially in enhancing pharmacological activity by participating in hydrogen bonding interactions with the receptors. In continuation to this a series of twenty new pyridine containing 1,3,4-oxadiazole heterocycles were synthesized and characterized by analytical techniques like ^{1}H NMR, ^{13}C NMR, IR and Mass spectrometry. The synthesized compounds were screened for their antimicrobial activity by serial broth dilution method. From the results, compounds with electron withdrawing group found to possess excellent antibacterial activity. They were further screened for antitubercular activity against mycobacterium tuberculosis *$H_{37}Ra$* (ATCC 25177) and *M. BCG* (ATCC 35734) strains by XTT assay method and they were found to possess excellent antitubercular activity.



P-235

Novel Nano Formulation For Treatment Of Age-Related Macular Degeneration

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Abstract: Age-related macular degeneration is the leading cause of blindness. It is caused due to deterioration of the central portion of the retina that is the macula. The macula is the central vision of the eye that record the images and sent to the brain via the optic nerve.There are two basic types of age-related macular degeneration: “dry” and “wet.” Approximately 85% to 90% of the cases of age-related macular degeneration are the “dry” (atrophic) type, while 10-15% are the “wet” (exudative) type.Currently, only intravitreal injections are available for the treatment of age-related macular degeneration. The injection therapy is painful and difficult to administer along with limitations such as need to administer every month. Therefore need the development of a novel formulation for the treatment of age-related macular degeneration.The topical route is the most frequent and preferred way to deliver drugs to the eye. There are several conventional formulations and therapies that available for the treatment of ocular diseases however due to the unique anatomy and physiology of the eye, efficient ocular drug delivery to the posterior segment is very challenging.The ocular bioavailability of drugs at the posterior segment of the eye is very poor. Conventional treatments, such as eye drops, ointment, injections and implants, either suffer from low bioavailability (Less than 5 %), systemic side effects, toxicity, dose dumping or hypersensitivity.Recently novel drug delivery systems play an important role in the treatment of age-related macular degeneration. The sustained release drug delivery through suitable Nano formulation(liposome, Solid lipid Nanocarrier, Implants, In_situ implants, depot formulations)system maybe minimize the dose frequency and improve bioavailability during the treatment of age-related macular degeneration.

P-236

"Studies on bioactive heterocyclic compounds containing 1,3,4-oxadiazole moeity and their antimicrobial activity"

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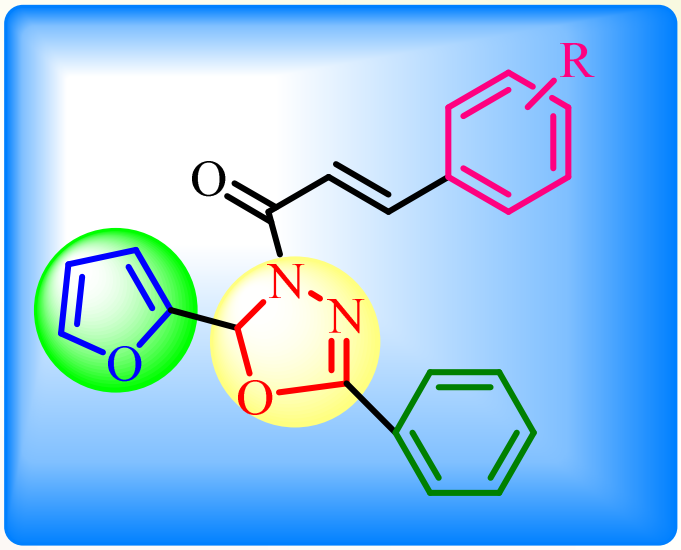
Abstract: In a search of novel fused heterocycles having high activity and with low toxicity, a series of compounds containing furan and 1,3,4-oxadiazole rings were designed and synthesized by a three-step synthetic route starting from furan-2-carbaldehyde and benzohydrazide. The structures of all the synthesized compounds were confirmed by ^{1}H NMR, ^{13}C NMR, mass spectrometry and elemental analysis. All the synthesized compounds have been evaluated for their *in vitro* antimicrobial activity against four bacterial strains *Staphylococcus aureus* (MTCC 96), *Streptococcus pyogenes* (MTCC 442), *Escherichia coli* (MTCC 443), *Pseudomonas aeruginosa* (MTCC 1688), fungal strains like *Candida albicans* (MTCC 227), *Aspergillus niger* (MTCC 282) and *Aspergillus clavatus* (MTCC 1323) using serial broth dilution method. From the results, it was found that compounds with electron withdrawing group exhibited excellent antibacterial activity while compounds with electron donating group showed very good antifungal activity.



P-237

Synthesis and antimicrobial activity of quinazoline clubbed 4-thiazolidinone hybrid heterocycles

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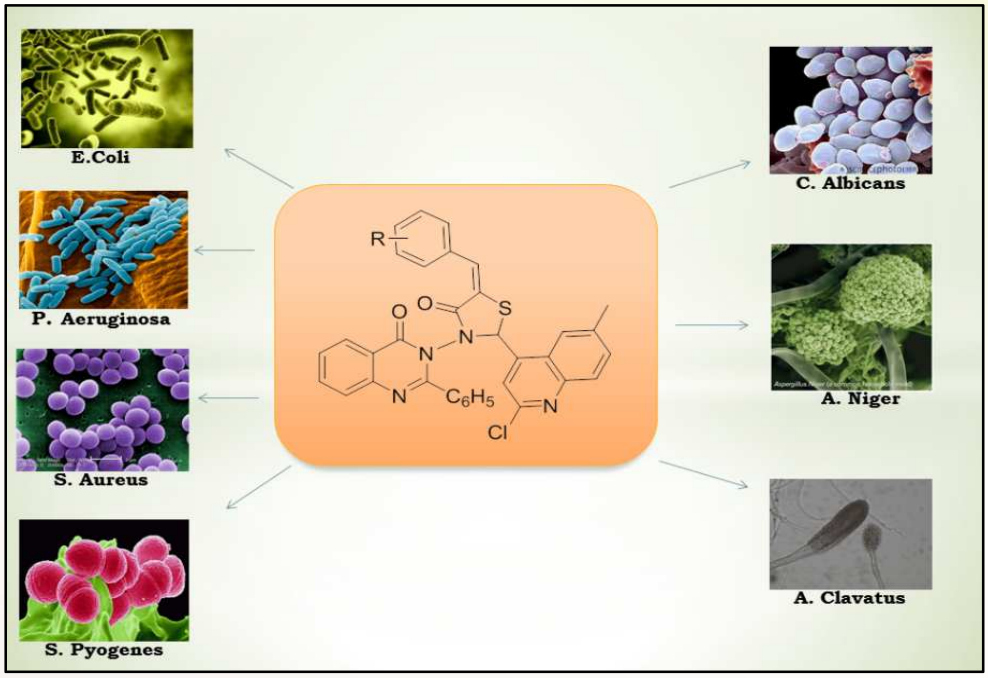
Abstract: The age-old drug therapy found to be ineffective against drug-resistant microbial pathogens and has lent additional urgency in medicinal chemistry. In continuation to this, the synthesis of novel series of structurally related 4-thiazolidinone and quinolones derivatives is described. A series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



P-238

Synthesis and antimicrobial activity of 1,3,4-oxadiazole based heterocyclic compounds"

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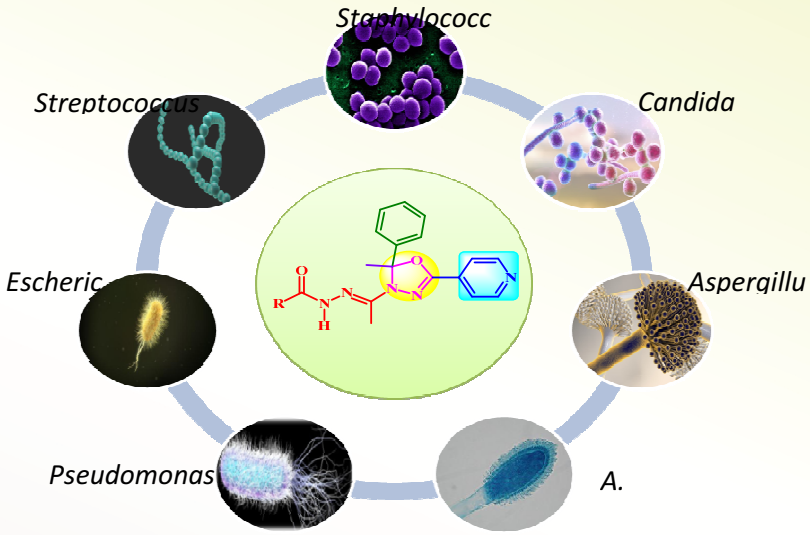
Abstract: A Series of 1, 3, 4-oxadiazole derivatives were preciselysynthesized and characterized by IR,^{1}H NMR,^{13}C NMR spectroscopy and mass spectrometry. The novel synthesized *N*'-(1-(2-methyl-2-phenyl-5-(pyridin-4-yl)-1,3,4-oxadiazol-3(2*H*)-yl)ethylidene)benzohydrazides were screenedfor their *in vitro* antimicrobial activity against four bacterial stains like *Staphylococcus aureus* (MTCC-96), *Streptococcus pyogenes* (MTCC-442), *Escherichia coli* (MTCC-443), *Pseudomonas aeruginosa* (MTCC-1688), and three fungal *Candida albicans* (MTCC 227), *Aspergillus niger* (MTCC 282), *A. clavatus*(MTCC 1323) by using conventional broth micro dilution method. It was our observation that the presence of electron withdrawing groups at *para* position of phenyl ring extremely enhanced the antibacterial activity. The antimicrobial screening data revealed that selected screened compounds (HC_1-5, HC1-10, HC_1-1, HC_1-4, HC_1-8, HC_1-17) exhibited significant activity against all microbial and fungal strains.



P-239

New scaffold of 4-oxo-thiazolidine derivatives as potent anti-microbial agents

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ABSTRACT: A new series of 4-oxo-thiazolidine has been synthesized and compounds **5_{a-j}** have been charectrized by various techniques like IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. All the newly synthesized compounds have been screened against four bacterial strains: *Staphylococcus aureus*, *Streptococcus Pyogenus*, *Escherichia Coli*, *Pseudomonas aeuinosa* and two fungal pathogens: *Candida albicans* and *Aspergillus clavatus*. The results have been expressed as minimal inhibition concentration (MIC µg/mL) in comparison with standard drugs. Compounds **5a,5c,5d,5e** and **5i** show moderate to good activity against selected bacterial strains (MIC=62.5µg/mL to 125µg/mL). *In vitro* antitubercular activity study of newly synthesized compounds **5_{a-j}** has been carried out against *Mycobacterium tuberculosis* H_{37}Rv. Two compounds **5c** and **5j** have shown good antituberculosis activity in comparison with standard drugs.

P-240

Sustainable and green protocols for C-S, C-P and P-Chalcogenides Bond Formations

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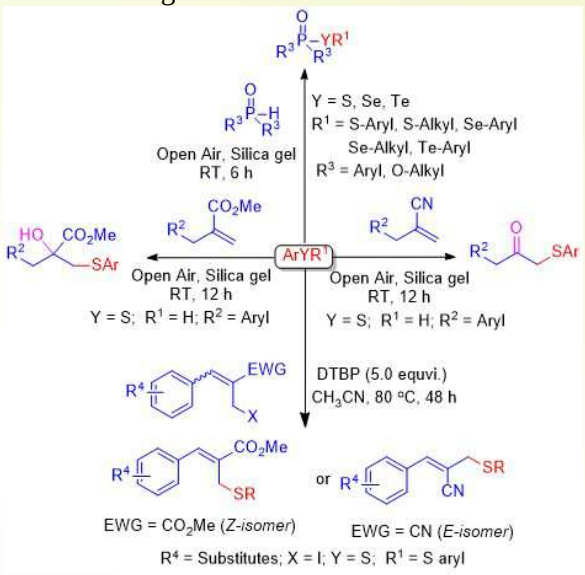
Abstract: Due to their ubiquitous importance in organic synthesis, pharmaceuticals, materials, medicinal chemistry, and agrochemicals, the development of novel sustainable protocols for the synthesis of organochalcogenides and organophosphorus moieties have attracted much attention in recent yeras.[1] Traditionally, these molecules were synthesized via transition metal-catalyzed cross-coupling reactions.[1] In recent years, synthetic organic chemists are looking for suitable alternatives to traditional transition-metal catalysts for the synthesis of these molecules. This abstract will provide the detailed discusion on the recently developed green organic methods by our research group for the construction of C-S, C-P, and P-Chalcogenide bonds.[2]



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P-241

Recent Advances in TBHP (tert-butyl hydro peroxide)-Promoted Cross -Coupling Reactions

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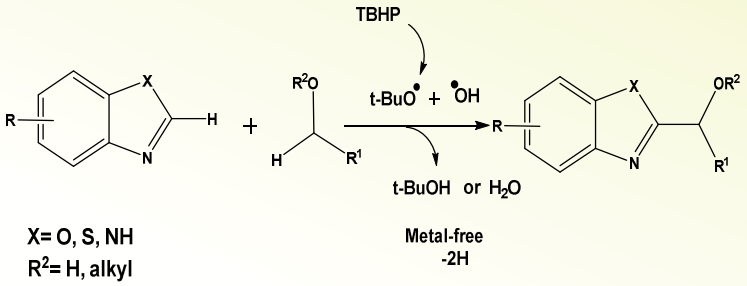
Abstract: DTBP and TBHP have recently been used in a variety of radical processes either in the presence or absence of transition metals for C-C, C-N, and C-S cross-coupling reactions.[1]Mostly, such transformations proceed*via* radical mechanism. In this abstract, we provide a brief review on the oxidative coupling of azoles with ethersunder metal- free and solvent-free conditions. [2]Initially, the alkoxyl radical, which is generated from a homolytic cleavage of TBHP, abstracted a hydrogen atom from the -position C–H bond of benzothiazole and ethanol and then forms the corresponding free radicals. Finally, carbon-carbon bond formation via termination of two radicals afforded the desired cross-coupling product. More importantly, this procedure is a very simple and powerful green protocol for the alkylation of heteroarenes.



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P-242

Chiral Mn(III) salen complexes as a catalyst for the Asymmetric epoxidation of styrene

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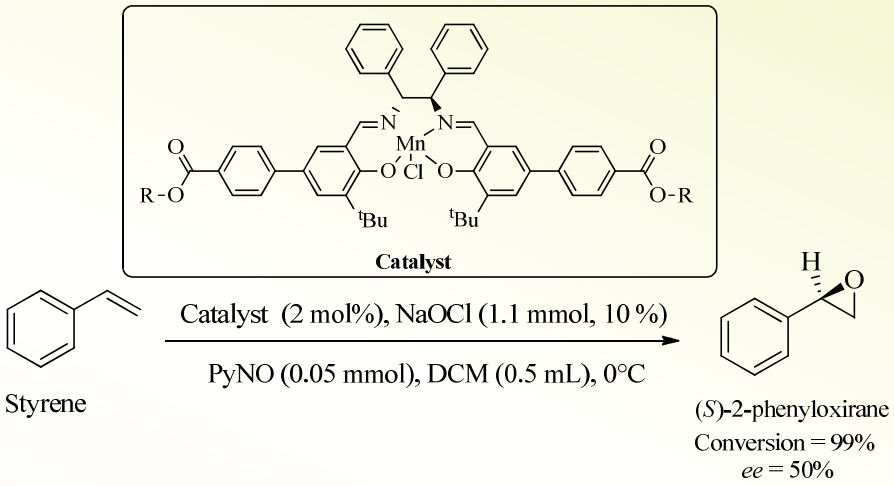
Abstract: The development of method for the synthesis of enantiomerically pure epoxides is considered to be one of the most interesting fields of asymmetric catalysis [1]. Among several catalytic strategies of formation of enantio-pure epoxides, the asymmetric epoxidation of non-functionalized alkenes catalyzed by chiral Mn(III) salen complexesis considered to be the most effective strategy[2].Chiral Mn(III) salen complexes was firstly developed by Katsuki and Jacobsen and utilized in the enantioselectiveepoxidation of unfunctionalized olefins[3-4]. By considering this, we have synthesized different chiral Mn(III) salen complexes and used in asymmetric epoxidation of styrene. The asymmetric epoxidation of styrene, catalyzed chiral Mn(III) salen complexes (2mol%)with NaOClafforded the (*S*)-2-phenyloxirane in 99% yield with 50% *ee* in the presence of pyridine N-oxide (0.05 mmol) in dichloromethane at 0°C.



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P-243

N-Aryl Imine Pd(II) Complex as an Efficient Precatalystfor Heck Reaction

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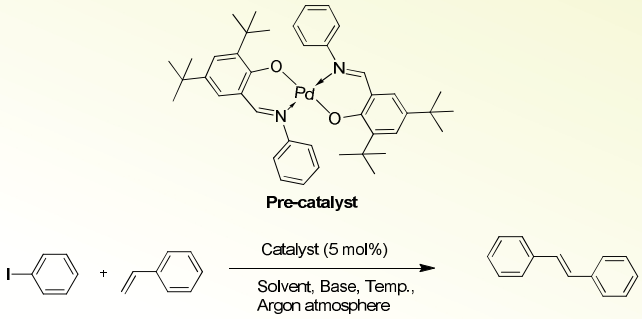
Abstract: Transition metal complexes ofsalen ligands are knownfrom many years, but their design and synthesis still stimulate interestin diverse fields of science[1-2]. Heck reaction of unsaturated halide (or triflate) and alkenes catalyzed by palladium metalgivingsubstituted alkenes [3].These products are used in the synthesis of natural products, pharmaceutical intermediates, conducting polymers, pesticides, and liquid crystals [4-5].We have synthesized N-aryl imine Pd(II) complexesfrom palladium acetate and bidentateligands which are derived from 3,5-ditertbutylsalicyaldehyde and derivatives of aniline. These complexes were characterized by FT-IR, ^{1}H-NMR, ^{13}C-NMR, HRMS, CHNS and single crystal X-ray.These Pd(II) complexes were applied in Heck reaction for the synthesis of stilbene by using styrene and iodobenzenein DMF and $NaHCO_3$ as a base at 140 ^{o}C and stilbene was obtained in 99%.



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Synthesis and characterization of novel Schiff base ligand of 5-bromoisatin with phenylhydrazine and its complexation with Ni(II)

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Abstract: Isatin is one of the most bioactive compounds exhibiting different biological activities. In our present work we have synthesized Schiff base ligand of 5-bromoisatin with phenylhydrazine by conventional method that is used as ligand (L). Above synthesized ligand acts as good complexing agent due to azomethine group (C=N) and plays a significant role in medical and pharmaceutical fields. Further Schiff base ligand was employed for complexation with Ni(II) by conventional thermal method and microwave assisted techniques as well. The characterization of above synthesized ligand and complex were carried out by elemental analysis, molecular weight determination, magnetic moment measurement and various spectroscopic techniques (UV- Vis, FTIR, NMR etc.). Purity of compounds was checked by Silica –Gel TLC.

Keywords; Schiff base ligand, 5-Bromoisatin, Phenylhydrazine, Thermal method, Spectroscopic techniques

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ENTHALPY-ENTROPY COMPENSATION (EEC) EFFECT IN REDOX KINETICS BETWEEN PARA-SUBSTITUTED ANILINE AND PEROXOMONOSULFATE IN ACIDIC MEDIUM

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Abstract: Peroxoacids are potential oxidizing agents of considerable significance. Peroxomonosulfate is a hydrolytic product of peroxodisulfate and it is considered to be much better oxidant than its parent analogue. we are also engaged with studies of kinetics of peroxomonosulfate oxidations[1-7] Peroxomonosulfate oxidation of some para-substituted aniline in aqueous perchloric medium has been studied and leads to the formation of azoxybenzene-4-4'-disulfonic acid from Sulfanilic Acid[8]. The reaction was under second order conditions. The reaction is retarded by hydrogen ions. Various thermodynamics parameters have been reported in this study to investigate the nature of the reaction mechanism in solutions. Therefore, Isokinetic relationship and exner's equation are useful to arrive at a decision whether or not a common mechanism is operative for a series of reactions. Also, the Isokinetic parameter β is further useful in deciding whether or not the system is enthalpy controlled or entropy controlled.

Keywords: Compensation, Enthalpy, Entropy, Isokinetic Temperature, Oxidation.

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Recent Advances in Asymmetric Aza-Michael reaction: A Brief Review

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Abstract: Chiral nitrogen-containing organic molecules display interesting biological activities and are important synthons [1]. Asymmetric aza-Michael reaction provides a facile and versatile method for obtaining such compounds. It has been possible to induce asymmetry in these reactions by using various chiral auxiliaries and adopting different strategies. Asymmetry can be induced in the Michael reaction by following different strategies:

(a) By using an appropriate Michael acceptor that is bonded to a chiral auxiliary.
(b) By using chiral nitrogen nucleophiles.
(c) By using chiral ligands in stoichiometric amount during the reaction.
(d) By using chiral catalysts.

In order to illustrate the above strategies, we focused specifically on the different methodologies reported for performing stereocontrolled aza-Michael reactions. The examples were classified on the basis of the mode of asymmetric induction (*e.g.*, external induction/non-covalent interaction or internal induction/covalent bond formation), the roles in reactions (as a solvent or catalyst), and their structural features (*e.g.*, imidazolium-based chiral cations, other chiral oniums; proline derivatives). introduction of the initial chirality source, that is, in relation to the use of the chiral auxiliary methodology either incorporated at the acceptor or at the nitrogen nucleophile, the use of chiral ligands or the use of asymmetric catalysis conditions.

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3. the roles in reactions (as a solvent or catalyst), and their structural features (e.g., imidazolium-based chiral
4. cations, other chiral oniums; proline derivatives).

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Regioselective 1,3-Dipolar Cycloaddition Reaction of Unsymmetrical Pyridinium Ylides under Mild Conditions

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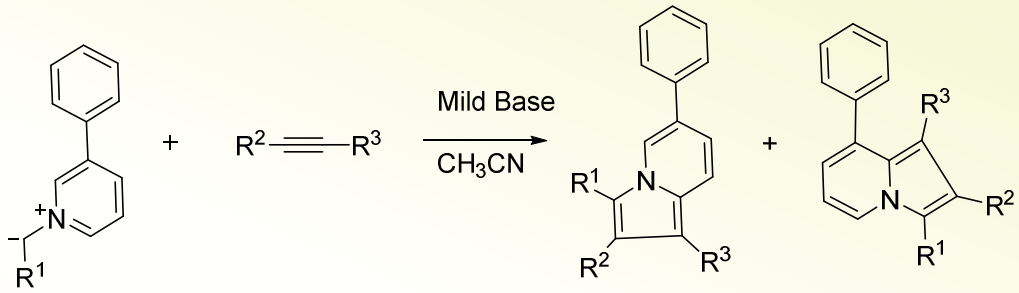
Abstract: 1,3-Dipolar cycloaddition reaction of pyridinium ylides is a widely applied method for the synthesis of Indolizine derivatives. The later being bicyclic bridgehead nitrogen heterocycles having interesting biological activities and fluorescence properties. We have made an effort to synthesize a library of unsymmetrically substituted indolizine derivatives under milder conditions without using any oxidizing agent. In the present study a series of reactions incorporating [3+2]cycloaddition on 3-phenylpyridinium ylide with variety of symmetrical as well as unsymmetrical electron deficient dipolarophiles have been carried out. Interesting observations pertaining to various compositions of regioisomers have been made. Auto-aromatisation of the cycloadduct under milder conditions has been achieved. The experimental yield of the products is sufficient and spectroscopic techniques - ^{1}H-NMR, ^{13}C-NMR and HRMS have been used for characterization of products.



Nanocrystals: A Promising Topical Formulation Strategy for the Treatment of Atopic Dermatitis

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Abstract: Atopicdermatitis (AD) is a common, chronic, relapsing, inflammatoryskin disease that primarily affects young children and adults too.Statistic says that it affects up to 20% of children and up to 3% of adults.The prevalence of AD is increasing day by day, and literature shows rising number of patients suffering from AD during the past decade.Topical treatment of skin diseases is vastlystriking, dueto reduction in the attainable systemic drug concentrations and thus systemic side effects ascompared to the conventional (parenteral or oral) drug administration.Topical corticosteroids and calcinurin inhibitors are currently used in form of ointment and creams for treatment of Atopic dermatitis. Amongst all these topical therapies, corticosteroids are preferred drugs but potent steroids causes hypertrophy of the skin, where topical calcinurin inhibitors have bioavailability and skin irritation issues. This strongly indicates need to develop suitable formulation, which could cure the same. Novel formulation development strategies of these drugs like solid Lipid Nanoparticles (SLN), Nano Lipid Carriers (NLC), Micremulsion, Nanoemulsion, Liposomal gel, Hydrgels have been studied and reported. As a solution to the current problems, nanocrystal may be explored as they are crystals of 100% pure drug, improves solubility and thereby bioavailability and minimizes the risk of incompatibility with excipients also. Thus present review envisage the potential of nanocrystals,their application, challenges and future scope in topical drug delivery.

Key words: Atopic dermatitis, topicalformulation strategies, nanocrystals, novel formulations

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3D Printing by Hot-Melt Extrusion; New Era for Development of Personalized Medicines and continuous manufacturing of pharmaceuticals

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Abstract: Continuous manufacturing of pharmaceutical products is an essential industrial application for cost-cutting and time-saving. Design and development of fabricated therapeutic products for superior properties and modified release using 3D printing are emerging fields. Organ and tissue printing is a very growing application of 3D printing. This technique is very promising for the development of novel personalized pharmaceuticals.3D printing is a simple, robust, and cost-effective technique for developing pharmaceutical products. It allows the costume design and dose adjustment as per the requirement of the patient (Personalized drug dosage forms).The hot-melt extrusion traditionally used for the enhancement of solubility of poorly soluble drugs. However 3D printing using hot-melt extrusion is a recent technology for the development of novel pharmaceutical dosage forms. It works on the principle of the melted polymer where deposited layer by layer in a predefined manner.Fused disposition modeling isa leading 3D technique used in the continuous manufacturing of pharmaceuticals and it works on the basis of hot-melt extrusion. This filament of printing material is where loaded into the heated nozzle followed by the deposited layer on the printing table. It is applicable for a wide range of printing material and having the capacity to the printing of matters with required shape. Fused disposition modeling can be used for the manufacturing of films, tablets, implants etc. In the feature,the personalized dosage is a new era of medicine and manufacturing of pharmaceuticals using 3D printing hot-melt extrusion technology.

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Iron Oxide Nanoparticles: For Cancer Treatment

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Abstract: While cancer is one of the world's most hazardous and second most lethal diseases, present conventional treatment is not extremely inadequate in terms of success rate of treatment or the quantity of side effects. Therefore, treatments with better results are extremely desirable. Thanks to latest development in the synthesis of high-quality inorganic nanoparticles, there are increasing numbers of types of nanoparticles (NPs) available for therapeutic, diagnostic and theranostic applications.Iron oxide NPs (IONPs) are an innovative tool that is ideal for innovation and practical execution as they offer remarkable potential for biomedical application in the fields of therapy, diagnosis, theranostics, toxicology and so on. This review focuses on summarizing some well-known facts about preparation methods, properties (Structural, mechanical, optical, electrical and magnetic), various sizes and shapes of IONPs and their controlling strategies. The review inculcates various therapeutic approaches such as stimuli-responsive delivery system, phototherapy, immunotherapy, biotherapeutic therapy, radiotherapy in the effective treatment of cancer. The review further includes various diagnosis modalities and strategies for effective cancer diagnosis and treatment. The review also focuses on summarizing some well-known facts about pharmacokinetics, biosensing, toxicity. The review also includes distinguished facts of iron involvement in ferroptosis for the treatment of cancer. In addition, molecular dynamic study of IONPs, iron based organometallic polymers and polymeric stents are also discussed.

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EXPLORATION AND APPLICATION OF COLD ATMOSPHERIC PLASMA AS HAND SANITIZER

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Abstract: In last few years cold atmospheric plasma (CAP) application has been researched in field of medicine, agriculture, food packing and cosmetics. CAP can be produced by passing inert gas or mixture of gasses in high voltage electric field where outer most electrons is pulled off from atoms and molecule of gas. Electrons of CAP has higher temperature then to ions and neutrals. CAP is comprised of ions, electrons, and free radicals of gases used in generating plasma. CAP is promising alternative for low temperature sterilization as it is suitable for most of the surfaces and it require very less time for sterilization. There are many ways to produce plasma but it is restricted parameters which can have effect on its sterilization effect.

In the presented work we have used plasma jet where gas is discharged between high power electrodes, and plasma is formed. This plasma pushed outside in the form of jet. We also have isolated and identified bacteria from hands of different volunteers who are using sanitizer or disinfections frequently and tested against different commercially available hand sanitizers and soaps and some of the bacteria shows resistance towards sanitizing chemicals. We have mainly focused on optimizing dose of plasma jet for safe use and killing of bacteria. Our study is focused on pseudomonas aeruginosa (P. aeruginosa) and Staphylococcus aureus (S. aureus) as both are isolated from the hand and are frequent contaminant in hospitals and resistant to many antibiotics.

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