ISCBC-2014

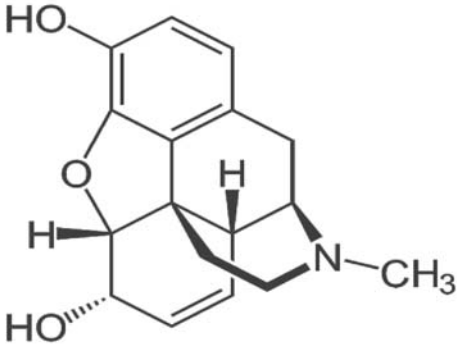
20th ISCB International Conference
on
Chemistry and Medicinal Plants in Translational Medicine for Healthcare

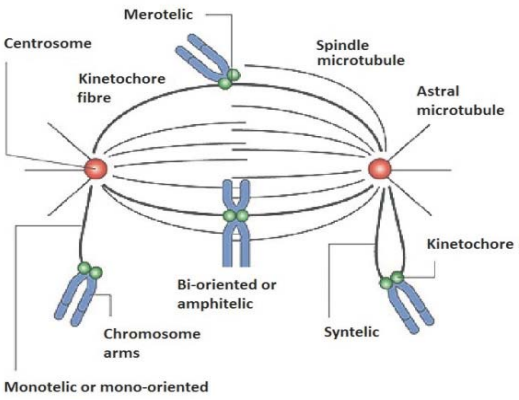
Organized by

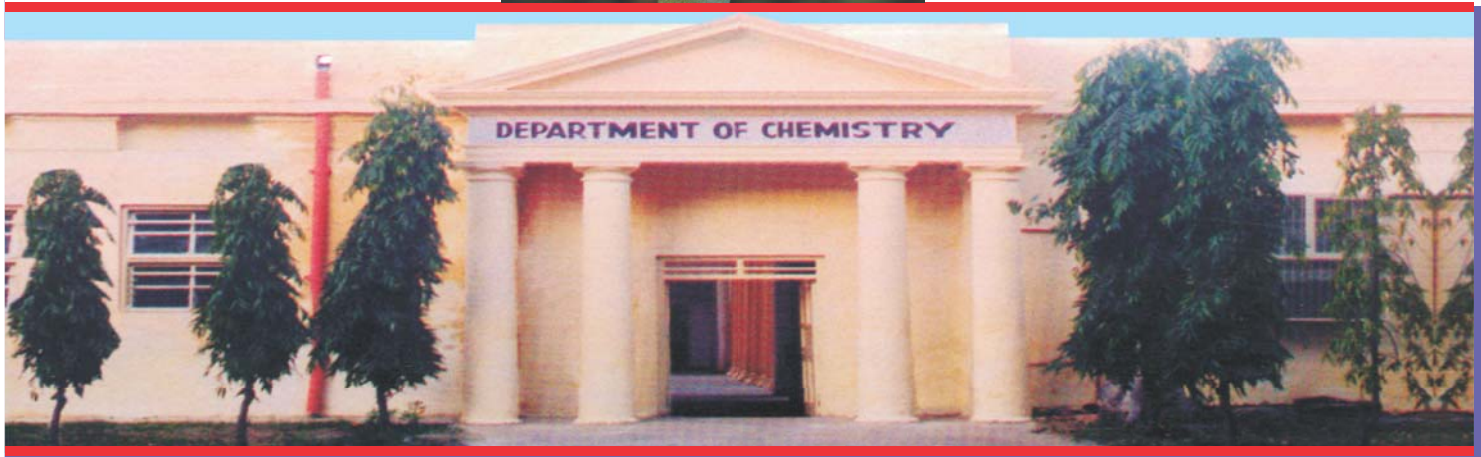
Department of Chemistry, University of Delhi

1st - 4th March 2014

BOOK OF ABSTRACTS







Venue:

The University Conference Centre
Opposite Botany Department, University of Delhi
Delhi-110 007

Sponsored by

1. Council of Scientific and Industrial Research, New Delhi
2. Defense Research and Development Organization, New Delhi
3. Department of Science and Technology, New Delhi
4. Indian Council of Medical Research, New Delhi
5. National Medicinal Plants Board, New Delhi
6. Petronet LNG Limited, New Delhi
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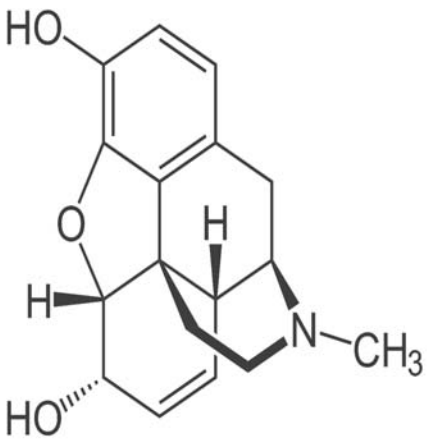

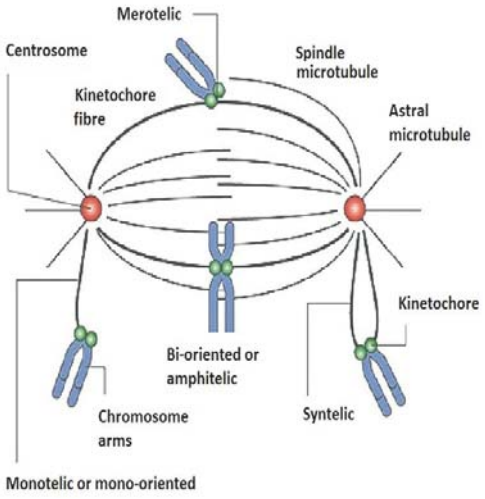

ABSTRACTS
SCIENTIFIC PROGRAMME

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University of Delhi

From the desk of
ISCB President and General Secretary

Prof. Anamik Shah **Dr PMS Chauhan**

Interdisciplinary interactions of researchers are of prime importance for the advancement of knowledge and applications of knowledge. Such interactions are much more important when come to drug research.The process of drug research has become more difficult, risky and expensive due to very tight regulatory parameters. To make a break through in this area a close interaction between the scientists and technologists in the area of chemistry and biology is highly desired. With this view in mind **Indian of Society Chemists and Biologists** is making consistent efforts to encourage interdisciplinary research activities in the field of chemistry and biology. **Indian Society of Chemists and Biologists** is unique in the sense that it promotes multidisciplinary research as compared to several scientific societies in the individual capacity with confined objectives. During the past the society has been very successful in achieving the targets.

We are extremely happy that its 20thISCB International Conference (ISCBC- 2014) on "**Chemistry and Medicinal Plants in Translational Medicine for Healthcare**" is being organized at Department of Chemistry, University of Delhi on 1st to 4th March, 2014. We are glad that the scientific committee is bringing out an abstracts book covering the presentations to be made during ISCBC-2014**.** 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 plenary lectures, invited lectures by the eminent scientists from India and abroad. 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 poster sessions. We are looking to the galaxy of speakers and young participants who made this conference a memorable event. We extend our warm welcome to all National and International delegates from pharmaceutical companies, research organization, universities and academic institutes wish them very happy stay at Delhi. Now Finally I take this opportunity to express my sincere thanks and gratitude to members and office bearers of organizing committee of 20th International Conference (ISCBC-2014).

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

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

MESSAGE

University of Delhi

20th ISCB International Conference
Department of Chemistry, University of Delhi
1 – 4 March 2014

Dear Delegates,

On behalf of the Organizing Committee and my own, I welcome the eminent scientists from India and abroad, research scholars, students and guests of the ISCB International Conference on "Chemistry and Medicinal Plants in Translational Medicine for Healthcare", organized by the Department of Chemistry, University of Delhi on 1 – 4 March 2014.

This is the second time that we are organizing ISCB International Conference at University of Delhi; first time it was organized in February 2009. We have invited eminent scientists working in the thematic areas of the conference for the benefit of the young participants and researchers working in the complementary areas of chemistry and biology. Participants will discuss and deliberate on areas of their research interests and expertise over four days beginning on 1 March, 2014. Besides the inaugural lecture, there will be fourteen plenary, forty eight invited and seven invited short lectures in the conference. Along with seventy podium presentations, there are two hundred ten posters, which will be presented in three different poster sessions during extended lunch breaks on the first, second and third days of the conference. The organizing committee of the conference has scheduled a Banquet Dinner for all the delegates and guests of the conference on 2 March 2014. The idea of the organization of Banquet Dinner is to provide ample opportunities to younger delegates to interact with the speakers who are renowned experts in their areas of research.

The organizing committee of the Conference has endeavoured hard to make the stay of all participants comfortable and enjoyable. Please do not hesitate to let the organizers know in case you need any assistance at any point during the conference.

MESSAGE

Professor Ashok K Prasad
Organizing Convener of the Conference
Department of Chemistry
University of Delhi
Delhi – 110 007
Ph: +91-11-27662486; (0)-9818131666

ISCBC - 2014

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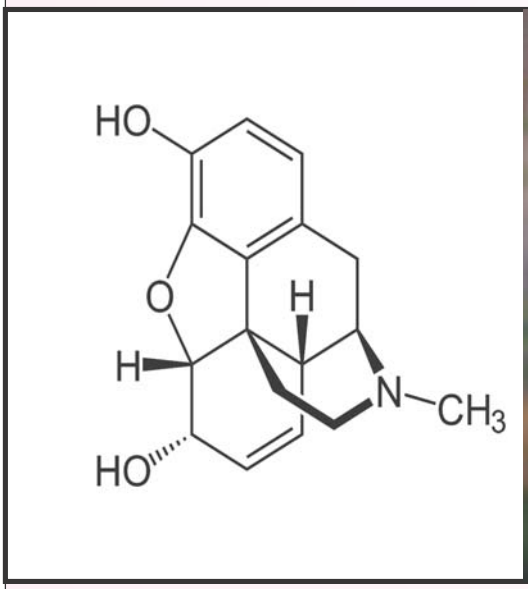

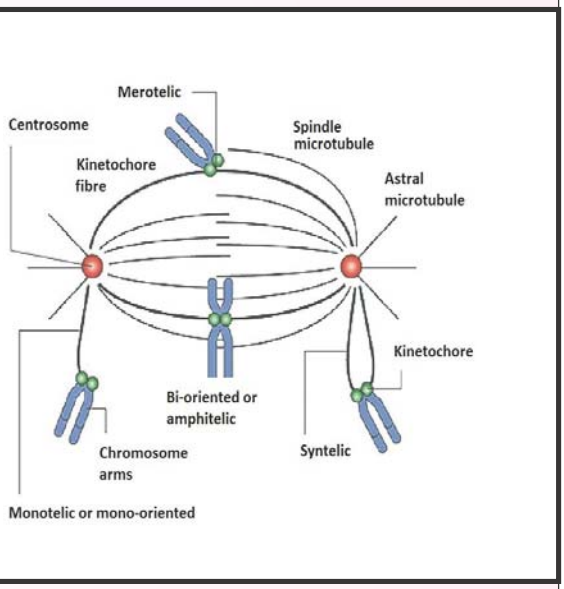

20th ISCB International Conference

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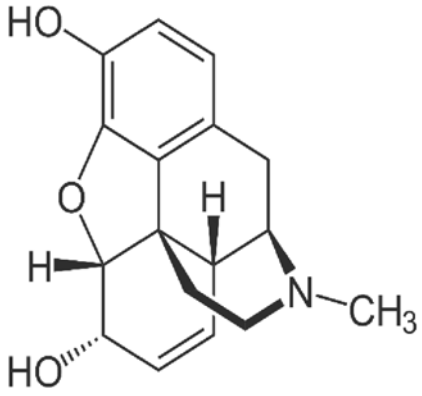
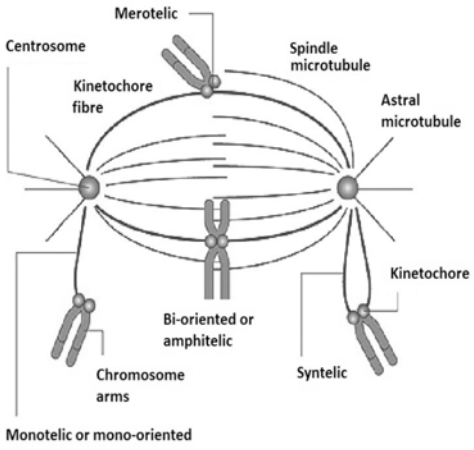
Scientific Programme





20th ISCB International Conference

SCIENTIFIC PROGRAMME

20th ISCB INTERNATIONAL CONFERENCE ON
Chemistry and Medicinal Plants in Translational Medicine for Healthcare
Department of Chemistry, University of Delhi
1st - 4th March 2014

Saturday, 1st March 2014

08.00 am – 09.15 am	**REGISTRATION**	
09.15 am – 10.45 am	**INAUGURATION AND INAUGURAL LECTURE**	
	Professor Goverdhan Mehta, *FRS* (*University of Hyderabad, India*) **Inaugural Lecture**	Enhancing Nature and chemical space through synergy between natural products and organic synthesis for human wellbeing
10.45 am – 11.15 am	**HIGH TEA**	
11.15 am – 01.10 pm	**TECHNICAL SESSION I** **Chairpersons: Professor VS Parmar and Professor Monika Datta**	
11.15 am – 11.55 am –	**Professor Dr Jesper Wengel** *(SDU, Denmark)* **PL – 1**	Locked and unlocked nucleic acids (LNA and UNA): Properties and applications
11.55 am – 12.25 pm	**Dr Souvik Maiti** *(CSIR-IGIB Delhi, India)* **IL – 1**	Silencing miRNA function: Opportunities and challenges
12.25 pm – 12.50 pm	**Professor Dr Rodolfo Lavilla** *(University of Barcelona, Spain)* **IL – 2**	Multi-component reactions with heterocycles: New possibilities in synthesis, application in medicinal chemistry and bio-imaging
12.50 pm – 01.10 pm	**Dr Jeetender Chug** *(IISER Pune, India)* **IL – 3**	Visualizing transient structures in A-site RNA of the ribosome: New structures of known molecules for drug target
01.10 pm – 02.40 pm	**LUNCH-CUM-POSTER SESSION – I**	
02.40 pm – 04.50 pm	**TECHNICAL SESSION II** **Chairpersons: Professor Gurmeet Singh and Professor RD Kaushik**	
02.40 pm – 03.20 pm	**Professor VK Singh**, *FNA* *(IISER Bhopal, India)* **PL – 2**	Enantioselective Michael reactions using 2-enyolpyridine-*N*-oxide as a template
03.20 pm – 03.50 pm	**Professor Javed Iqbal**, *FNA* *(ILS Hyderabad, India)* **IL – 4**	Synthesis of migrastatin analogues as potent cell migration inhibitors
03.50 pm – 04.10 pm	**Dr Pradeep Kumar** *(CSIR-NCL Pune, India)* **IL – 5**	Organocatalytic approach to enantiopure syn/anti-1,3-polyols/1,3-amino alcohols/1,3-diamines: Application to the synthesis of bioactive compounds
04.10 pm –	**Dr DK Mohapatra**	Novel synthetic methods: Towards the synthesis of

04.30 pm	*(CSIR-IICT Hyderabad, India)* **IL - 6**	complex natural products
04.30 pm – 04.50 pm	**Dr Amit Kumar** *(IIT Patna, India)* **IL – 7**	Exploration of acid-base catalysis concept in glycosidation
04.50 pm – 05.20 pm	**TEA/ SNACKS**	
05.20 pm – 07.35 pm	**TECHNICAL SESSION III** **Chairpersons: Dr GP Garg and Dr Sundeep Dugar**	
05.20 pm – 06.00 pm	**Dr SK Puri** *(CSIR-CDRI Lucknow, India)* **PL – 3**	Recent developments in drug discovery for malaria
06.00 pm – 06.30 pm	**Professor Dr Michael D. Threadgill** *(University of Bath, UK)* **IL – 8**	Potency and selectivity in the design and development of new tankyrase inhibitors
06.30 pm – 06.55 pm	**Professor Kohki Ebitani** *(JAIST, Japan)* **IL – 9**	Heterogeneous catalytic systems for transformations of biomass-derived materials into value-added chemicals
06.55 pm – 07.15 pm	**Dr P Venkatesu** *(University of Delhi, India)* **IL – 10**	Ammonium ionic liquids as biocompatible co-solvents for the structure and stability of biomolecules
07.15 pm – 07.35 pm	**Dr Anupam Bhattacharya** *(BITS Hyderabad, India)* **IL – 11**	4-Substituted pyrrolo[2,3-c]quinoline systems: Synthetic, anti-tubercular and selective metal detection studies
07.40 pm – 09.00 pm	**DINNER** **Venue: Dinning Hall, Conference centre**	

Sunday, 2nd March 2014

09.30 am – 11.15 am	**TECHNICAL SESSION IV** **Chairpersons: Professor Anshu Dandia and Professor SK Sharma**	
09.30 am – 10.10 am	**Professor Dr Rainer Haag** *(Free University Berlin, Germany)* **PL – 4**	Multivalent dendritic polyglycerol sulfates as highly anti-inflammatory and antiviral drugs
10.10 am – 10.35 am	**Professor Dr Rafael Luque** *(University of Cordoba, Spain)* **IL – 12**	Valorization of waste feedstocks to biomedically-relevant valuable end products
10.35 am – 10.55 am	**Dr AJ Varma** *(CSIR-NCL Pune, India)* **IL – 13**	Natural polymers in medical products: Carboxycelluloses and their nanoparticles
10.55 am – 11.15 am	**Professor Kazuaki Matsumura** *(JAIST, Japan)* **IL – 14**	Biomedical application of oxidized polysaccharide as a self degradable material
11.15 am – 11.45 am	**TEA/ SNACKS**	

11.45 am – 01.30 pm	**TECHNICAL SESSION V** **Chairpersons: Professor RC Rastogi and Professor DS Rawat**	
11.45 am – 12.25 pm	**Professor Ganesh Pandey**, *FNA (CBR Lucknow, India)* **PL – 5**	Enantiocontrolled construction of all carbon quaternary centre at C-3 position of cyclic amines: Application towards the total synthesis of alkaloids
12.25 pm - 12.50 pm	**Professor SMS Chauhan** *(University of Delhi, India)* **IL – 15**	Supramolecular chirogenesis in porphyrinoids and related compounds
12.50 pm – 01.10 pm	**Professor Dr Hamid Dhimane** *(Descartes University Paris, France)* **IL – 16**	Electromethoxylation of L-lysine derivatives towards biologically relevant natural compounds and analogs
01.10 pm – 01.30 pm	**Dr Arun K Sinha** *(CSIR-CDRI, Lucknow, India)* **IL – 17**	Towards protection group free step: Economical synthesis of some natural and non-natural bioactive polyphenolic compounds
01.30 pm – 03.00 pm	**LUNCH-CUM-POSTER SESSION – II**	
03.00 pm – 04.35 pm	**TECHNICAL SESSION VI** **Chairpersons: Dr VK Kansal and Dr CH Khanduri**	
03.00 pm – 03.15 pm	**Dr Indresh Kumar** *(BITS Pilani, India)* **SL – 1**	Organocatalytic cascade strategy for synthesis of small molecule natural products (SMNPs)
03.15 pm – 03.30 pm	**Dr Vineet Kumar** *(FRI Dehradun, India)* **SL – 2**	Structural analysis and functionalization of polysaccharides
03.30 pm – 03.45 pm	**Dr Rakesh Kumar** *(KMC University of Delhi, India)* **SL – 3**	New methodology for the synthesis of bicyclic heterocyclic systems from 1,4-dihydropyridines
03.45 pm – 04.00 pm	**Dr T Narender** *(CSIR-CDRI Lucknow, India)* **SL – 4**	Lead molecules from Indian medicinal plants for metabolic and infectious diseases
04.00 pm – 04.15 pm	**Dr Jyoti Singh** *(Sci-Edge Information Pune, India)* **SL – 5**	Natural product scaffold in drug discovery- A case study
04.15 pm – 04.25 pm	**Mr Vivek K Sharma** (*University of Delhi, India*) **SL – 6**	Chemo-enzymatic access to sugar modified nucleosides of biological importance
04.25 pm – 04.35 pm	**Mr U Chinna Rajesh** (*University of Delhi, India*) **SL – 7**	Development of nano-material as recyclable heterogenous catalysts in organic conversions
04.35 pm – 05.00 pm	**TEA/ SNACKS**	
05.00 pm – 07.15 pm	**TECHNICAL SESSION VII** **Chairpersons: Professor Rama Kant and Dr Niraj Shekhar**	
05.00 pm – 05.40 pm	**Professor Uday Maitra**, *FNA (IISc Bangalore, India)*	A pro-sensitizer approach for enzyme sensing using lanthanide luminescence in a hydrogel

	PL – 6	
05.40 pm – 06.10 pm	**Professor AK Singh** *(Allahabad University, India)* **IL – 18**	Retinoids and tocopherols in translational medicine: Design, synthesis and biological activity of compounds in vitamin A and E series
06.10 pm – 06.35 pm	**Professor Dr Xavier Coqueret** *(University of Reims Champiegne, France)* **IL – 19**	Radiation-induced micro- and nano-fabrication of polymer-based 3-D structures for microfluidics and life-science analytics
06.35 pm – 06.55 pm	**Dr Rajiv Sharma** *(PLS Mumbai, India)* **IL – 20**	Isocytosines as novel xanthine oxidase inhibitors
06.55 pm – 07.15 pm	**Dr Paul Servin** *(Nanopartica GmbH Berlin, Germany)* **IL – 21**	The development of a new biodegradable polymer for drug delivery applications: From start to well-known ending
07.45 pm – 10.45 pm	**BANQUET DINNER Venue: DROMI, Brig. SK Mazumdar Marg, DRDO Residential Complex, Timarpur, Delhi- 110 007**	

Monday, 3rd March 2014

09.30 am – 11.15 am	**TECHNICAL SESSION VIII Chairpersons: Professor JM Khurana and Dr PL Soni**	
09.30 am – 10.10 am	**Professor Tushar K Chakraborty,** *FNA (IISc Bangalore, India)* **PL – 7**	Ti(III)-mediated stereoselective radical reactions: Application in the synthesis of natural products
10.10 am – 10.35 am	**Dr Ahmed Kamal** *(CSIR-IICT Hyderabad, India)* **IL-22**	Podophyllotoxin congeners as potential anti-cancer agents
10.35 am – 10.55 am	**Professor Dr Patrick J Guiry** *(University College of Dublin, Ireland)* **IL-23**	Recent developments in catalytic asymmetric synthesis
10.55 am – 11.15 am	**Dr Anil Kumar** *(BITS PIlani, India)* **IL-24**	Transition metal-catalyzed C-H functionalization and tandem reactions for synthesis of imidazo[1,2-]pyridine based heterocyclic compounds
11.15 am – 11.45 am	**TEA/ SNACKS**	
11.45 am – 01.30 pm	**TECHNICAL SESSIONS IX Chairpersons: Professor Rita Kakkar and Professor Pawan K Sharma**	
11.45 am – 12.25 pm	**Professor Dr Christophe Len** *(UTC Compiegne, France)* **PL – 8**	Water as green solvent in organic chemistry
12.25 pm – 12.50 pm	**Professor Bhishma K Patel** *(IIT Guwahati, India)* **IL – 25**	Unpredictable coupling reactions

12.50 pm – 01.10 pm	**Dr Rajneesh K Misra** *(IIT Indore, India)* **IL – 26**	Optical limiting performance of donor-acceptor molecular systems
01.10 pm – 01.30 pm	**Dr Ravi P Singh** *(IIT Delhi, India)* **IL – 27**	Asymmetric vinylogous reactions: A powerful tool for creating functionalized framework
01.30 pm – 03.00 pm	**LUNCH-CUM-POSTER SESSION – III**	
03.00 pm – 04.40 pm	**TECHNICAL SESSION X** **Chairpersons: Professor SC Jain and Professor AK Gupta**	
03.00 pm – 03.40 pm	**Dr Rajesh Gokhale**, *FNS (CSIR-IGIB Delhi, India)* **PL – 9**	Chemico-cellular rewiring in mycobacteria
03.40 pm – 04.00 pm	**Professor Michele Vittadello** (*Medgar Evers College Brooklyn, USA*) **IL – 28**	Enhanced oxygen evolution from photosystem II coupled to chemically modified graphene
04.00 pm – 04.20 pm	**Professor Anamik Shah** *(Saurashtra University Rajkot, India)* **IL – 29**	Exploration of new scaffolds as promising anti-inflammatory and anticancer agents
04.20 pm – 04.40 pm	**Dr Dalip Kumar** *(BITS Pilani, India)* **IL – 30**	Indole-based heterocycles as novel inhibitors of tubulin polymerization
04.40 pm – 05.00 pm	**TEA/ SNACKS**	
05.00 pm – 07.35 pm	**TECHNICAL SESSION XI** **Chairpersons: Professor RK Sharma and Professor AK Mishra**	
05.00 pm – 05.40 pm	**Dr Ram A Vishwakarma** *(IIIM Jammu, India)* **PL – 10**	Discovery and development of anticancer NCEs: Targeting clinically validated kinases
05.40 pm – 06.10 pm	**Professor Dr Erik Van der Eycken** *(University of Leuven, Belgium)* **IL – 31**	Cationic gold-catalyzed heteroannulations
06.10 pm – 06.35 pm	**Professor MP Kaushik** *(DRDO-DRDE Gwalior, India)* **IL – 32**	Quest for new antidotes against toxicants
06.35 pm – 06.55 pm	**Professor GS Chauhan** (*HP University Shimla, India*) IL - 33	Enzyme immobilized on nanogels as triggered drug delivery
06.55 pm – 07.15 pm	**Professor N C Desai** *(Bhavnagar University, India)* **IL – 34**	Flourine containing compounds – A new class of anti-infective agents
07.15 pm – 07.35 pm	**Professor AK Goswami** *(Mohanlal Sukhadia University Udaipur, India)* **IL – 35**	Biologically active metal chelates with special emphasis on hydroxytriazenes
07.45 pm –	**Dinner**	

09.30 pm	**Venue: Dinning Hall, Conference centre**	

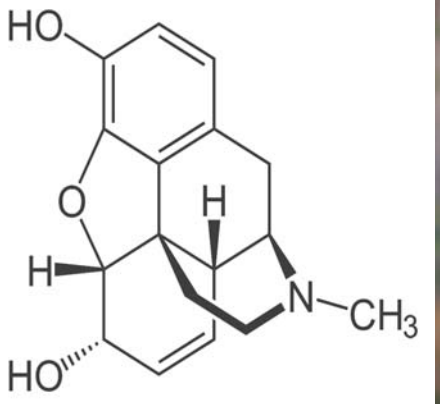
Tuesday, 4th March 2014

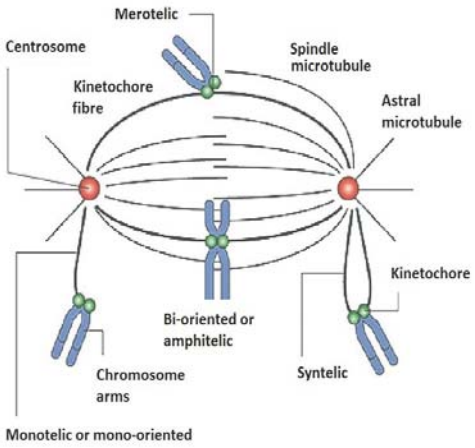
09.30 am – 11.15 am	**TECHNICAL SESSION XII** **Chairpersons: Professor MSM Rawat and Dr Nirada Devi**	
09.30 am – 10.10 am	**Professor VS Chauhan**, *FNA (ICGEB Delhi, India)* **PL – 11**	Development of blood stage vaccines against *P. falciparum* and *P. vivax*
10.10 am – 10.35 am	**Professor Dr Johan Van der Eycken** *(Gent University, Belgium)* **IL - 36**	A modular approach to chiral imidates: A new class of nitrogen-based chiral ligands as tools for medicinal chemistry
10.35 am – 10.55 am	**Dr PMS Chauhan** *(CSIR-CDRI Lucknow, India)* **IL - 37**	Synthesis of bioactive hybrid molecules as novel therapeutic agents
10.55 am – 11.15 am	**Dr Rajeev Gupta** *(University of Delhi, India)* **IL - 38**	Organic transformations by designed inorganic catalysts
11.15 am – 11.45 am	**TEA/ SNACKS**	
11.45 am – 01.30 pm	**TECHNICAL SESSIONS XIII** **Chairpersons: Professor Pawan Mathur and Professor RK Saxena**	
11.45 am – 12.25 pm	**Professor Rup Lal**, *FNA (University of Delhi, India)* **PL – 12**	Production of rifamycin analogs by genetic manipulation of rifamycin polyketide biosynthetic gene cluster of *Amycolatopsis mediterranei*
12.25 pm – 12.50 pm	**Professor Binghe Wang** *(Georgia State University, USA)* **IL – 39**	Bacterial SecA as a target for the development of antimicrobial agents
12.50 pm – 01.10 pm	**Dr Anil Kumar Dwivedi** *(CSIR-CDRI Lucknow, India)* **IL – 40**	Studies on herbal medicament, a new anti-stroke agent
01.10 pm – 01.30 pm	**Professor VK Tandon** *(Lucknow, India)* **IL – 41**	Natural product framework synthesis: Expeditious concise synthesis of dibenzo[b,d]oxepines, dibenzo[b,d]thie-pines and benzo[b]pyrano[2,3-d]oxepines through C-C insertion and ring transformation reactions
01.30 pm – 02.30 pm	**LUNCH**	
02.30 pm – 04.20 pm	**TECHNICAL SESSION XIV** **Chairpersons: Dr Sudershan Kumar and Dr A Chakraborty**	
02.30 pm – 03.10 pm	**Dr Balaram Ghosh**, *FNA (CSIR-IGIB Delhi, India)* **PL – 13**	A novel cinnamate derivative attenuates bronchial epithelial injury and asthma features in mouse model

03.10 pm – 03.40 pm	**Professor Timothy Egan** *(University of Cape Town, South Africa)* **IL – 42**	Exploring heme as a target for antimalarials
03.40 pm – 04.00 pm	**Dr Vibha Tandon** *(University of Delhi, India)* **IL – 43**	DMA a bisbenzimidazole: An odyssey of a small molecule as radioprotectant
04.00 pm – 04.20 pm	**Dr Rachna Sadana** *(Houston, USA)* **IL – 44**	Cytotoxic coscinamide analogues inhibit tubulin polymerization and cause cell death *via* apoptosis
04.20 pm – 04.40 pm	**TEA/ SNACKS**	
04.40 pm – 06.40 pm	**TECHNICAL SESSION XV** **Chairpersons: Professor RA Mane and Professor Jibon Kotoky**	
04.40 pm – 05.20 pm	**Professor Dr Jyoti Chattopadhyaya** *(Uppsala University, Sweden)* **PL – 14**	Therapeutic potential of carba-LNA modified oligonucleotide to control the phosphate degradation of target RNA by harnessing the relative hydration
05.20 pm – 05.45 pm	**Professor NG Ramesh** *(IIT Delhi, India)* **IL – 45**	Natural products to natural products and their mimics
05.45 pm – 06.05 pm	**Professor SK Kukreti** *(University of Delhi, India)* **IL – 46**	DNA structural polymorphism: A biologically relevant phenomenon
06.05 pm – 06.25 pm	**Dr JK Saxena** *(CSIR-CDRI Lucknow, India)* **IL – 47**	Plasmodium falciparum purine nucleoside phophorylase (PfPNP): A potent drug target
06.25 pm – 06.40 pm	**Mr Manish Omprakash** *(Buchi Labortechnik AG, Switzerland)* **IL – 48**	BÜCHI solutions for regulated pharmaceutical industries
06.40 pm – 07.40 pm	**POSTER PRIZE DISTRIBUTION AND VALEDICTORY SESSION**	
07.40 pm – 09.00 pm	**Dinner** **Venue: Dinning Hall, Conference Centre**	

ISCBC - 2014

Inaugural Lecture





20th ISCB International Conference

Professor Goverdhan Mehta, *FRS*
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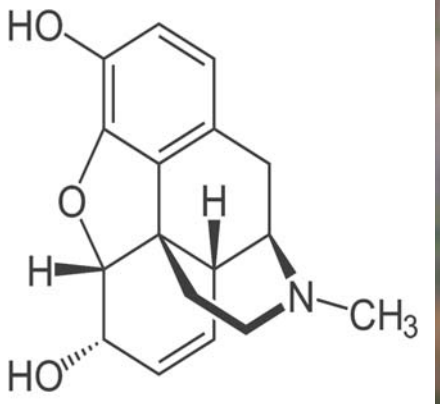
Enhancing Nature and Chemical Space through Synergy between Natural Products and Organic Synthesis for Human Welbeing

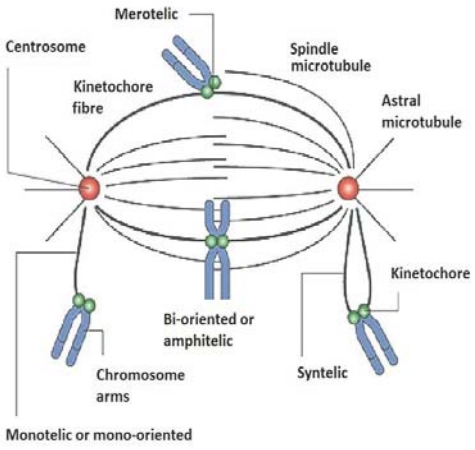
Nature, the master craftsman of molecules, has created almost an inexhaustible array of molecular entities, inherently endowed with drug-like attributes due to evolutionary memories compiled in a complex biological environment. There is little surprise therefore that many natural products display potent, wide ranging and at times unique biological activity profile and have served as inspirational platforms for exploring new chemical space and drug discovery. The presentation would highlight the intrinsic synergy between natural products, total synthesis and drug discovery through some recent examples. In particular, the focus will be on the development of 'global' strategies for total synthesis from our group that provide access to a whole family of natural products rather than a single entity for further biological evaluation and development. Efficacy of diversity oriented organic synthesis (DOS) in such endeavors will be highlighted.

INAUGURAL LECTURE

ISCBC - 2014

Plenary Lecture





20th ISCB International Conference

Professor Dr Jesper Wengel
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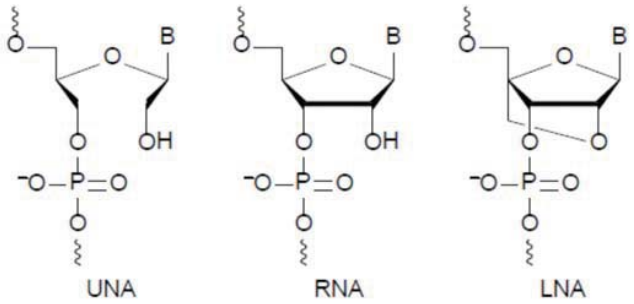
Locked and Unlocked Nucleic Acid (LNA and UNA): Properties and Applications

Whereas LNA (locked nucleic acid) increases binding affinity of probes against DNA and RNA targets, UNA (unlocked nucleic acid) is an acyclic form of RNA that reduces binding affinity. LNA and UNA therefore in many ways can be considered antipodes within the arsenal of synthetic RNA mimics. In the lecture it will be discussed how LNA and UNA modification of oligonucleotides, siRNA constructs and aptamers can lead to novel and appealing properties. For a rencent review, see M. A. Campbell and J. Wengel, *Chem. Soc. Rev.* 2011, *40*, 5680.



PLENARY LECTURE

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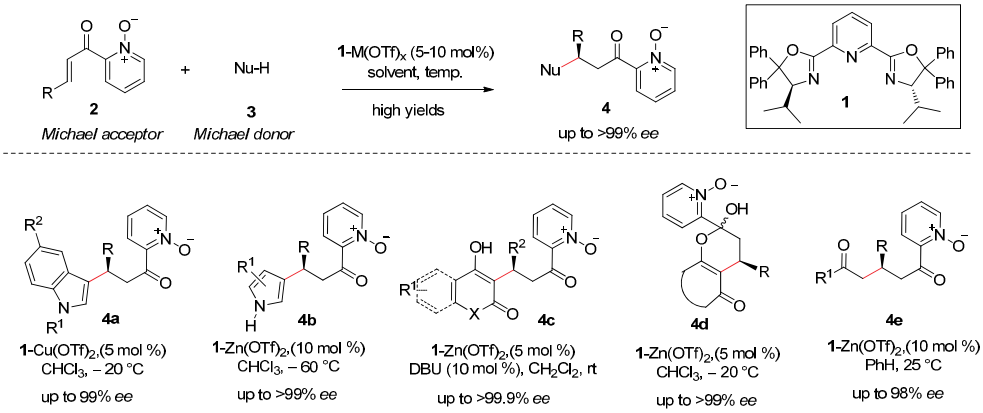
Enantioselective Michael Reactions Using 2-Enyolpyridine-*N*-Oxide as a Template

Michael reaction is one of the most fascinating and fundamental C-C bond forming reactions and has wide utility in organic synthesis. The asymmetric version of this reaction provides access to enantioenriched functionalized adducts from numerous Michael acceptors and donors. Several bidentate chelating substrates such as nitrostyrenes, β,γ-unsaturated α-ketoesters, alkylidene malonates, glyoxylates, pyruvates, acyl phosphonates, 2-acyl imidazoles, α'-hydroxy enones and other acyl heterocyclic compounds have been utilized in various enantioselective Michael reactions. In this context, bidentate chelating substrate 2-enoylpyridine *N*-oxide has recently been identified as a new template for the enantioselective Michael addition reaction in our group and others.[1,2]



Scheme: 2-Enoylpyridine *N*-oxide as a Template for Enantioslective Michael Reactions.

In this lecture, I will be focusing on our contribution towards the enantioselective Michael reactions of indoles,[1a] pyrroles,[1b] dialkyl malonates,[3a] 4-hydroxy coumarins,[3b] and 1,3-dicarbonyls[3c] and Mukaiyama-Michael using sillylenolethers,[3d] onto the 2-enoylpyridine *N*-oxides and their synthetic utility as important enantioenriched intermediates.

References:

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PLENARY LECTURE

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Recent Developments in Drug Discovery for Malaria

Malaria continues to be the most important parasitic infection ranking among the major health challenges for tropical and subtropical countries. The current failure to control malaria through effective treatment results mainly because of the under estimation of burden of disease owing to drug resistance and the widespread use of ineffective drugs. One of the underlying factors which favored the rapid development of cross resistance is the sharing of the same quinoline ring in the majority of synthetic antimalarials. Preservation of clinical utility of chloroquine had been a significant concern and challenge for several years. Building on leads from a traditional Chinese medicine, artemisinine the isolated active principle as well as several of its oil and water soluble first generation derivatives like artemether, arteether and artesunate have shown promise to meet dual challenge of treating drug resistant parasites as well as to check the rapid progression of fatal malaria infections. The loss of effectiveness of artemisinin and its derivatives to drug resistance would constitute a major disaster in the fight against malaria. Evidence from Southeast Asia shows that resistance to this class of antimalarials is likely to occur in future. The last few years have seen the development of innovative novel leads which have potential to be effective against multi-drug resistant parasites. For new medicines to be optimal in malaria control, they must also be able to reduce transmission through vector mosquitoes and inhibit the dormant liver stage hpnozoite forms. Chemoprophylaxis as a malaria control strategy also needs more intensive inputs since such agents would be significantly useful in preventing the spread of drug resistant malaria. Sustained investment over the next decade in discovery and development of new molecules is essential to enable the long term delivery of the medicines needed to combat malaria.

PLENARY LECTURE

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Multivalent Dendritic Polyglycerol Sulfates as Highly Anti-Inflammatory and Antiviral Drugs

Application of polymer therapeutics in medicine is a rapidly moving field that is gaining fast acceptance and recognition as an independent area of research and scientific endeavor.[1,2] The combination of a high density of end groups and a compact well defined molecule structure makes dendritic architectures attractive for biomedical applications. The synergy between their multivalency and size in nanoscale provides a range of options for chemical "smartness" along their molecular scaffold to achieve environment sensitive modalities.[3]

Due to their low degree of molecular weight dispersity, flexible design, and biocompatible nature, dendritic polyglycerols (PGs) have a broad range of potential applications in medicine and pharmacology.[4] The versatility of the polyglycerol scaffold for application in the biomedical field has been recently reviewed.[5]

Dendritic polyglycerol architectures have already been demonstrated to be useful in therapeutic approaches related to multivalency because of the synergy between the nano-sized dimensions combined with the high density of functional groups.[6,7] A challenging approach to the application of multivalent interactions is the mimicry of functional biomacromolecules with therapeutic relevance. Several attempts have been made to mimic specific glycoarchitectures, (i) the neutral species with hydroxyl end groups represents a good analogue of polysaccharides, and (ii) polyanionic derivates present similar activities to negatively charged polysaccharides, e.g., heparin, polysialic acid. The highly anti-inflammatory properties of the polyanionic systems make them interesting candidates for targeting rheumatic arthritis (RA).[8]

Results and Discussion

Most recently, our group demonstrated that polyanionic, dendritic polyglycerol sulfates (dPGS) exert strong binding affinity to cellular targets involved in the inflammatory process by inhibiting leucocyte infiltration *in vivo*.[7] We have further demonstrated that dPGS acts as a novel type of synthetic nanocarrier suited for inflammation-specific molecular imaging. Translation into the diagnostic application was accomplished by *in vivo* fluorescence imaging in a rat rheumatoid arthritis model, demonstrating fast and highly selective targeting of tissue inflammation.[8] In a recent study we compared the diagnostic potential of a NIR-dye-labeled system and the therapeutic efficacy of dPGS in RA.

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PLENARY LECTURE

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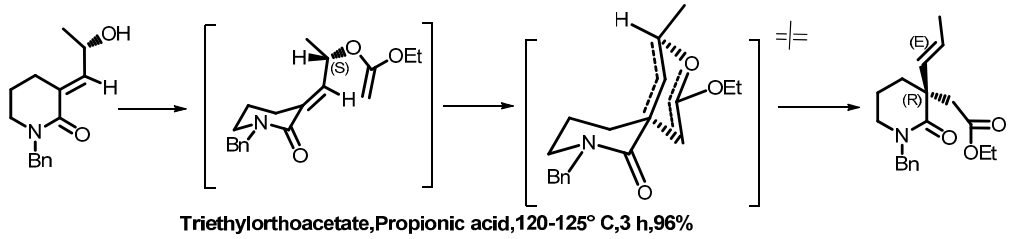
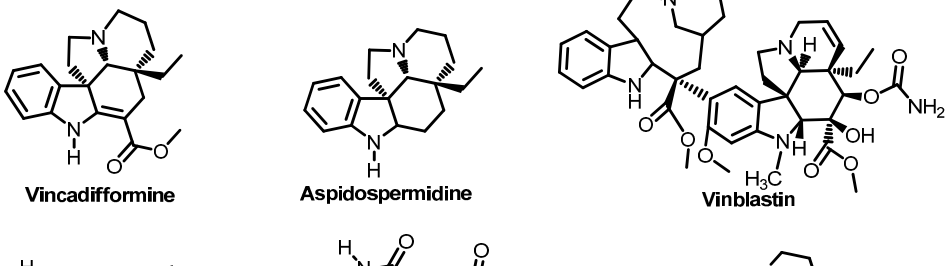
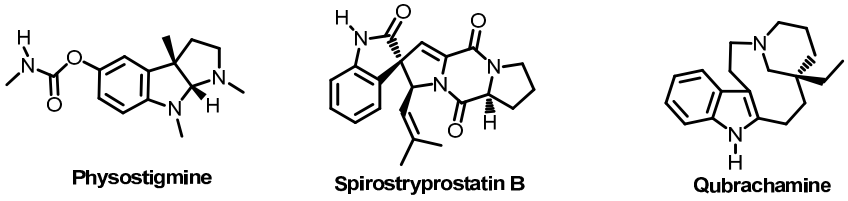
Enantiocontrolled Construction of all Carbon Quaternary Centre at C-3 Position of Cyclic Amines: Application towards the Total Synthesis of Alkaloids

Enantioselective construction of all carbon quaternary centres at C-3 position of lactams is an important and challenging transformation in organic synthesis. There are large numbers of biologically active alkaloids which contain all carbon quaternary centres at C-3 carbon of fused pyrollidine, piperidine and oxindole ring systems. Our ongoing interest in the total syntheses of biologically active alkaloids, motivated us to develop a general route to prepare key heterocyclic motif having all quaternary carbon centres at C-3 position as a possible precursor. In this context, we have developed a general and concise strategy for the construction of all carbon quaternary centre via [3,3]-sigmatropic rearrangement in high yield as well as enantiomeric excess.







Details of the concept and total synthesis of few alkaloids would be discussed.

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PLENARY LECTURE

Professor Uday Maitra, ***FNA***
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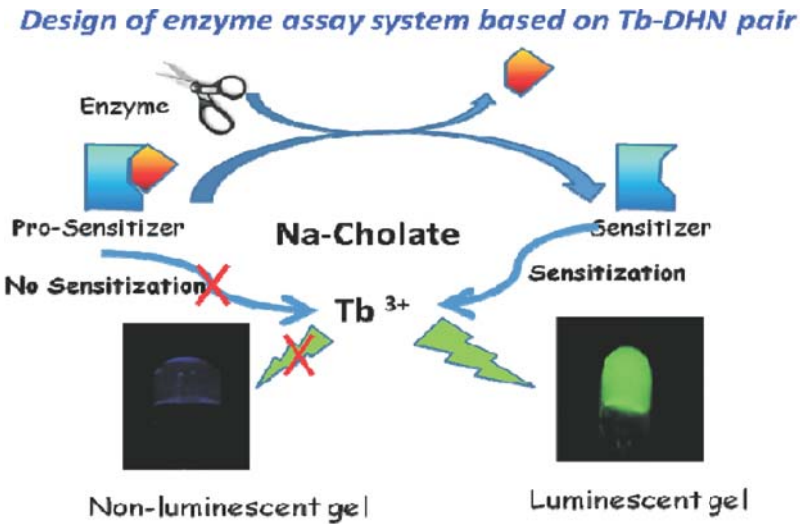
A '*pro*-sensitizer' Approach for Enzyme Sensing Using Lanthanide Luminescence in a Hydrogel

There are a number of substrate-based methods available for the sensing and assay of enzymes. These methods typically produce different types of outputs for different enzymes, depending on the type of the assay employed.

We have recently reported a sensitizer based enhancement of lanthanide luminescence through the self-assembly of multiple components in a metallohydrogel. Using this protocol, we have developed a '*pro-sensitizer*' based sensing of a number of enzymes. The advantage of this method is that all enzymes are sensed by the same output, *viz*, the green (or red) photoluminescence of Tb^{3+} (or Eu^{3+}) which is induced only when the enzyme is present, and may be observed using an inexpensive, hand-held long-wave UV lamp. The design of this enzyme sensing methodology will be highlighted in this lecture with a number of examples.



PLENARY LECTURE

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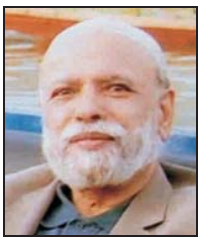

PLENARY LECTURE

Ti(III)-Mediated Stereoselective Radical Reactions: Application in the Synthesis of Natural Products

Development of efficient methodologies and their application in the synthesis of natural products sum up the very essence of organic synthesis.[1] The practice of the chemical synthesis of structurally complex molecules will fascinate organic chemists as long as they keep discovering new synthetic methods. The methodology developed by us for the synthesis of chiral 1,3-diols by radical-mediated opening of 2,3-epoxy alcohols using cp_2TiCl[2] has been successfully employed to construct the 1,3-diol moieties in many biologically active polyketide natural products.[3] The salient feature of this reaction was the chiral induction during the quenching of the intermediate radical center. A useful extension of this reaction led to the construction of quaternary chiral centres.[4] Subsequently, we showed that intramolecular trapping of the intermediate radical by a suitably positioned α,β-unsaturated ester moiety in the same molecule can give rise to carbocycles,[4] oxacycles[5] and azacycles.[6] Applications of these reactions in the synthesis of various natural products[7-10] will be discussed.

References:

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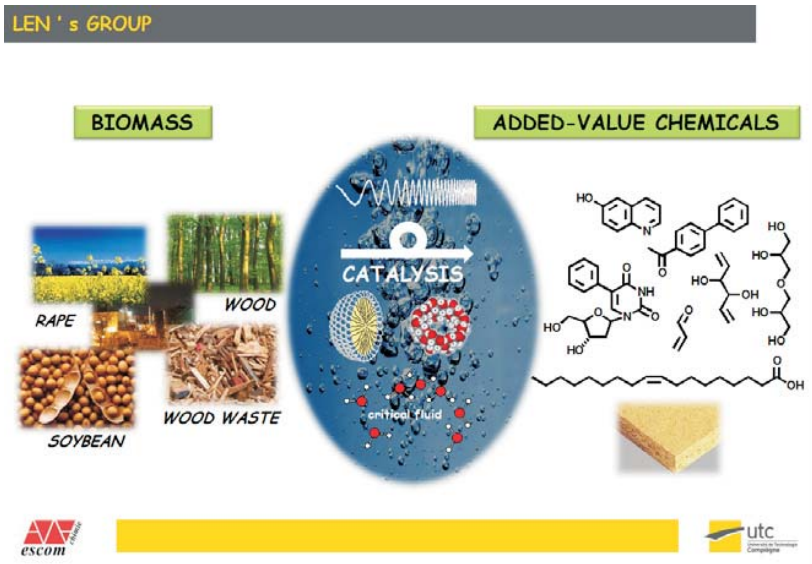
Water as Green Solvent in Organic Chemistry

According to the green chemistry principles, organic chemists are deeply encouraged to develop environmentally-benign products and processes using ecologically friendly materials and solvents, with no or minimal amount waste generation. In this context, water has emerged as a versatile solvent for organic chemistry in recent years. Water as a solvent is not only inexpensive and environmentally benign, but also gives completely new reactivity. Several green chemistry approaches using water as green solvent were developed for broad applications such as synthesis of biological compounds from carbohydrates and chemical modification of biomolecules. These approaches include: (i) green synthesis of quinoline derivatives in sole water using microwave irradiation and high temperature/pressure; (ii) green synthesis of biaryl compounds using the cross coupling Suzuki-Miyaura reaction in pure water using Natural Phosphate, cyclodextrin as a phase transfer agent; (iii) green synthesis in photo-switchable micellar system. Conception, synthesis and physico-chemical will be detailed.



PLENARY LECTURE

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Chemico-Cellular Rewiring in Mycobacteria

The bacterial genomic information has enhanced systems level understanding of bacterial physiology giving insights into perturbed metabolic interactions. The cross-talk between altered metabolic pathways and chemico-cellular changes in the cell leads to adaptive physiological functions. The challenge at this stage is to combine NGS analysis, both genomic and transcriptomic that can reveal biology of the organism. Our group has revealed mechanistic and regulatory interactions which culminate into biological outputs like community morphogenesis of Mycobacteria and its adaptation into novel intracellular niches to establish extra- pulmonary forms of infection. In this talk, I will provide perspective on the two aspects of chemico-cellular rewiring in Mycobacteria.

PLENARY LECTURE

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Discovery and Development of Anticancer NCEs: Targeting Clinically Validated Kinases

Since the discovery of phosphatidylinositol (PI) mediated signal-transduction and glycosylphosphatidylinositol (GPI) mediated membrane anchoring of specialized cell-surface proteins, the biology of PI/GPIs has remained in focus. A number of key cellular events (trans-membrane signaling, proliferation, vesicular traffic, chemotaxis, glucose-homeostasis and the membrane organization) are mediated by PI/GPIs with the involvement of specific biosynthetic and regulatory kinases and phosphatases. The pharmacological and clinical validation of phosphatidylinositol 3-kinase (PI3K) and downstream targets AKT and mTOR has provided new targets for discovery of specific kinase inhibitors for cancer and autoimmune diseases. The structural complexity and biological function of PI/GPIs present substantial challenges, and despite the efforts of several groups, their synthesis remains a difficult undertaking; complicated further by the structural and functional differences among the species and significant micro-heterogeneity in their lipid and glycan domains. In our efforts on chemical biology of PI/GPI molecules and drug discovery, we designed new and efficient approaches for the synthesis of the full-length GPI molecules and their structural and functional mimics to address specific questions pertaining to the biosynthetic inhibition and plasma-membrane micro-domain (lipid-raft) organization. Our current focus is on the medicinal chemistry of PI3K/AKT/mTOR axis for cancer and autoimmune diseases, and stem cell renewal and differentiation. Some of our contributions will be discussed.

PLENARY LECTURE

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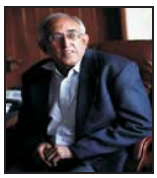

Development of Blood Stage Vaccines against P.falciparum and P.Vivax

An effective vaccine against Malaria, a major killer of children in the tropical world, has remained a scientific challenge. With the growing realization of potential value of vaccination as a strategy for malaria management and enhanced financial support vaccine development programmes have received a new lease of life. That is also fueled by a better understanding of the immune system, the effector mechanisms involved in protective immunity. Scientific challenges apart, real hurdles in the vaccine development are lack of laboratory correlates, a reliable animal model and difficulties in carrying out efficacy trials of candidate vaccines. However, a sporozoite stage malaria vaccine (RTS,S) has been cleared for Phase III trial, in Africa. We, at ICGEB, have been working on the development of blood stage vaccines against *Plasmodium falciparum* and *Plasmodium vivax*. A vaccine based on EBA-175 and MSP – 1 has completed its pre-clinical development and is being taken for clinical trials in humans. Development of vaccines against p.falciparum and p.vivax will be discussed in detail.

PLENARY LECTURE

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Production of Rifamycin analogs by Genetic Manipulation of Rifamycin Polyketide Biosynthetic Gene Cluster of *Amycolatopsis mediterranei*

Rifamycin B is an important antibiotic, produced by *Amycolatopsis mediterranei* S699. Semisynthetic derivatives of rifamycin B are used widely for the treatment of tuberculosis (*Mycobacterium tuberculosis*), leprosy (*Mycobacterium leprae*) and AIDS related mycobacterial infections. However, prolonged usage of this antibiotic has resulted in the emergence of resistant strains of *Mycobacterium tuberculosis,* the causative agent of tuberculosis. Due to chemical complexity of the rifamycin B molecule, so far, only six semi synthetic derivatives from rifamycin B could be produced. Although the rifamycin polyketide synthase (*rif*PKS) gene cluster, that synthesizes rifamycin B has collinear organization and was characterized in 1998, the manipulation of this gene cluster for the synthesis of rifamycin analogs was not an easy task. However, for the first time we demonstrated that *rif*PKS gene cluster can also be manipulated for the production of rifamycin B analogs by combinatorial biosynthetic approach. The efforts led to the swapping of acyltransferase (AT) domain of the sixth module (AT6) of rifamycin polyketide synthase (which adds propionate unit to the growing polyketide chain) with that of AT domain of the second module (AT2) of rapamycin PKS (*rap*PKS) (which adds acetate unit) in *Amycolatopsis mediterranei* S699. The resulting strain produced rifamycin derivative 24-desmethylrifamycin B which lacked the methyl group at C-33 of the rifamycin skeletal structure that was confirmed using NMR and LC-MS studies. The novel analog was further converted to 24-desmethylrifamycin S & 24-desmethylrifampicin, which were found to have a better antibacterial activity than rifamycin B. The drug testing analysis of the novel analog also confirmed its better activity (ten times) against multi-drug resistant strain of *M. tuberculosis*. This study has further opened up the possibility for further manipulations of *rif*PKS cluster by swapping other domains or inactivating modules for producing large number of rifamycin analogs for biological and pharmaceutical applications.

PLENARY LECTURE

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A novel Cinnamate Derivative Attenuates Bronchial Epithelial Injury and Asthma Features in Mouse Model

Airway epithelial injury is one of the key features in various respiratory diseases including bronchial asthma. It was hypothesized that improving epithelial injury could be an effective strategy for controlling these diseases.

We recently isolated and characterized a cinnamate derivative from *Piper longum*. Our subsequent structure-activity relationship (SAR) studies identified a novel cinnamate, ethyl 3′,4′,5′-trimethoxythionocinnamate (ETMTC), and it was found to be the most potent among various cinnamate derivatives synthesized in inhibiting inflammatory cell adhesion molecules (CAMs).

In this study, we investigated whether ETMTC could attenuate epithelial injury and ameliorate features of allergic asthma in a murine model. We observed that ETMTC treatment to ovalbumin sensitized and challenged mice reduced airway hyperresponsiveness (AHR), epithelial injury and airway inflammation. Further, mechanistic studies showed that ETMTC caused the reduction in the expressions of various CAMs, NF-κB activation, Th2 cytokines, eotaxin and 8-isoprostane. It also restores mitochondrial function in lung epithelial cells. These results suggest that ETMTC could be useful in developing efficient therapeutic molecule against asthma and other respiratory diseases.

PLENARY LECTURE

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Therapeutic Potential of Carba-LNA Modified Oligonucleotide to Control the Phosphate Degradation of Target RNA by Harnessing the Relative Hydration

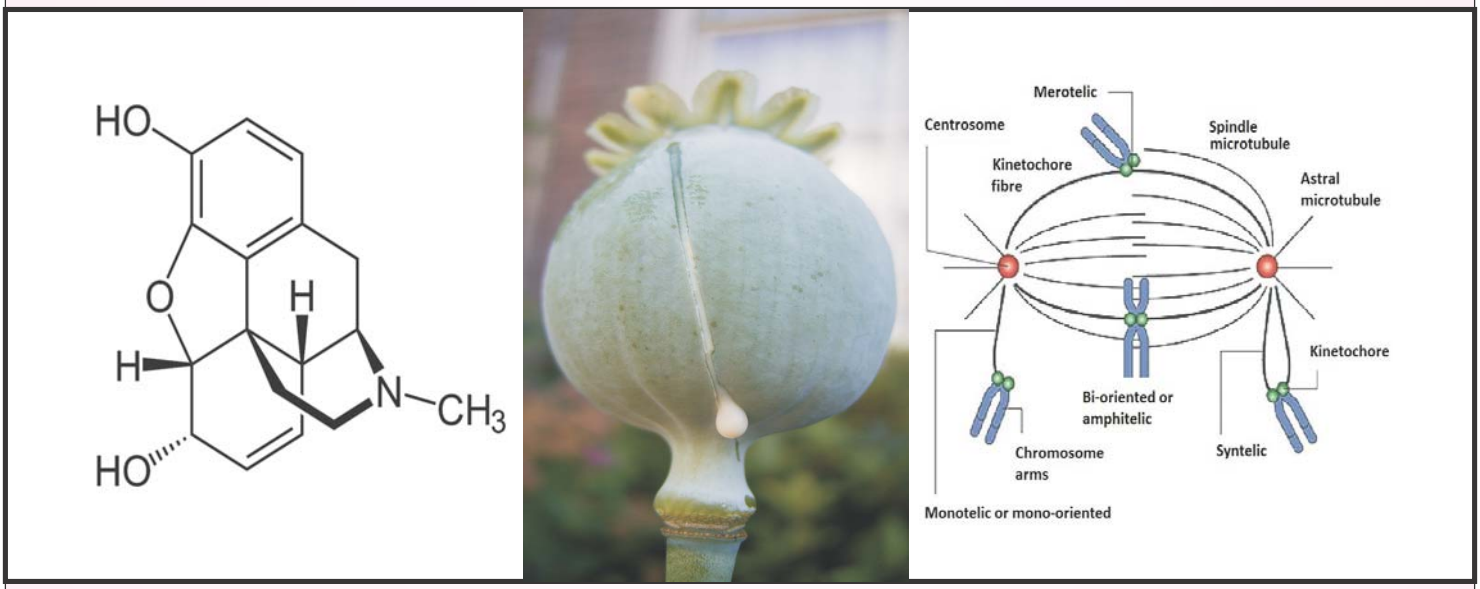
Ideal design of a therapeutic oligonucleotide requires that incorporation of chemical modification will impart correct nucleolytic stability and cell-penetration properties while binding to the target cellular mRNA and degrade it, preferably in a catalytic manner. Current understanding suggests that specific mRNA scaffold formation through its folding with the help of some cofactor, such as metal ion or a ligand, with or without an enzyme, which bring about the specificity of the phosphodiester bond cleavage in the mRNA in the ternary complex. For the degradation of the target mRNA with any of the endonucleases exploited in the antisense (ASO) or siRNA strategies require the stereochemical proximity of specific water molecules (active water) in the endonuclease-mRNA-ASO/siRNA complex. We will present compelling evidence that specific hydration level around phosphate ester change upon complexation and subsequent structure reorganization ensures acceleration of the mRNA cleavage/degradation. This presentation will address and provide some direct experimental evidence in support of the fact that water deprivation in the RNA duplexes retards its cleavage/degradation rate. A phosphodiester bond of target RNA do not cleave if there is no water around it. Using carba-LNA modified oligo, we have enhanced the cleavage rate of the target mRNA by 7-8-fold compared to the native counterpart by recruiting water.

For all relevant publications on carba-LNA see: www.boc.uu.se

PLENARY LECTURE

ISCBC - 2014

Invited Lecture



20th ISCB International Conference

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Silencing miRNA Function: Opportunities and Challenges

MicroRNAs (miRNAs) play crucial roles in regulating gene expression in many cellular contexts. Deregulation of miRNAs has been implicated in a number of disease conditions and thus, methods that can modulate mature miRNA levels in cells can have immense therapeutic potential. Classically miRNA knockdown has been carried out by usage of antisense oligonucleotides (antimiRs) against miRNA. Previously our lab has established the use of catalytic nucleic acid enzymes in the antagonism of miRNA. These also however are subject to the inherent drawbacks of systemic delivery. More recently, the use of small molecules in antagonism of miRNA has been tested by using synthetic libraries. Independently, we screened a library of well known aminoglycosides to test their inhibitory capacity to silence a model oncomir, miR-21. We found that streptomycin was able to do so by structural perturbation of the process of dicing giving it a potential new indication as an candidate anticancer agent. Further we developed a high throughput *in vitro* screening assay to identify small molecule inhibitors of miRNA maturation, and as proof of principle, we identified five potential inhibitors of another model oncomir miR-27a. Additionally, using rationally designed heterocyclic quinazoline based compounds and cyclic peptides, we explored the efficacy of small molecule mediated target specificity and discrimination. Conversely, we also provide evidence that aminoglycoside antibiotic usage can globally perturb miRNA function and thus be a potential cause of the observed drug toxicities paving way for the re-evaluation of use of RNA binding antibiotics in general. Particularly using a zebrafish model system, we posit that streptomycin can cause its well documented ototoxicity via direct perturbation of miR-96, miR-182 and miR-183 function.

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INVITED LECTURE

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Multi-component Reactions with Heterocycles: New Possibilities in Synthesis, Application in Medicinal Chemistry and Bio-imaging

New synthetic protocols arise from the use of fundamental *O*- and *N*-heterocycles as the key reactants in multicomponent reactions. Mechanistic variations over known processes are explored to develop new multicomponent reactions (Mannich- and isocyanide-type). The participation of cyclic enol-ethers, dihydropyridines and (benzo-fused)azines in these processes lead, in a straightforward manner, to a diverse set of complex drug-like compounds and these adducts constitute a new source of new chemical entities with interesting applications in medicinal and biological chemistry.

INVITED LECTURE

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Visualizing Transient Structures in A-site RNA of the Ribosome: New Structures of Known Molecules for Drug Target

Dynamic changes in RNA structure drive many essential processes in living cells. Studies of RNA dynamics have focused on fluctuations about the dominant ground state at sub-microsecond timescales or large-scale transformations in secondary structure occurring at timescales slower than seconds. By using NMR relaxation dispersion and mutagenesis, we show that non-canonical regions of A-site Ribosomal RNA undergo transient excursions away from the ground state towards short-lived (ms lifetimes) and low populated (2%) excited states that feature local rearrangements in secondary structure and base-pair alignment in regions rich in non-canonical residues. A-site ribosomal RNA contains two highly conserved internal loop adenines A1492 and A1493, which serve to decode the mRNA message by looping out and stabilizing a codonanticodon mini-helix when it is formed between mRNA and its cognate aa-tRNA. A-site is also known to bind to many antibiotics where drug binds the internal loop, flips the two adenines out and the adenines are forced to bind the codon-anticodon minihelix irrespective of correctness of tRNA. The excited state conformation we proposed is highly conserved and defines a new type of RNA switching that can be integrated into biological circuits. The A-site ES sequesters the A92 and A93 into base-pairs, such that they are no longer available for interacting with incoming tRNAs. Indeed, the C1407U mutation, which stabilizes the A-site ES has previously been shown to significantly increase the stop-codon readthrough and frame shifting, suggesting that the mutation weakens codon-anticodon interactions in the A-site and decreases the fidelity of elongating ribosomes.

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INVITED LECTURE

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Synthesis of Migrastatin Analogues as Potent Cell Migration Inhibitors

This presentation will describe our Studies directed towards Migrastatin family of Cell migration Inhibitors. The key synthetic step involves a Palladium catalyzed C-H activation leading to five and Six-member lactones which are manipulated to the core structure of Migrastatin and related analogs.

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INVITED LECTURE