

Residential School on Medicinal Chemistry and Drug Discovery and Development India
MCADDI 2015

Medicinal Chemistry and Drug Discovery and Development India

February 8-12, 2015

Sri Ramachandra University

Porur, Chennai, India

Forward:



It is a pleasure for me to welcome you to Medicinal Chemistry and Drug Discovery and Development India – 2015. The American Chemical Society (ACS) and the ACS Division of Medicinal Chemistry (MEDI) are pleased to be Co-Sponsors of this important course, along with the International Union of Pure and Applied Chemistry (IUPAC). We hope that you will find the course to be valuable, and that what you learn this week will help advance your career in drug discovery.

The American Chemical Society has a major goal to reach out to chemists in India to build new relationships for our mutual benefit. It is our hope that the participation of ACS and the MEDI Division in MCADDI 2015 will contribute to those efforts, and we are looking forward to productive interactions with you during the week, and in the future. We are confident that MCADDI 2015 will help to create the foundation for a future educational curriculum in Drug Discovery at Sri Ramachandra University and other universities in India.

A handwritten signature in black ink that reads "Diane Grob Schmidt".

Diane Grob Schmidt, Ph.D.

President, American Chemical Society

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Welcome to Medicinal Chemistry and Drug Discovery and Development India - 2015

Sri Ramachandra University and Pharma Innovation Sourcing Center LLC, USA are pleased to welcome you to MCADDI 2015, a 4.5-day Course co-sponsored by the American Chemical Society Division of Medicinal Chemistry and the International Union of Pure and Applied Chemistry (IUPAC), Division of Chemistry and Human Health. The successful program “Medicinal Chemistry India” held at Sri Ramachandra University in 2013 forms the basis for the 2015 program. However, MCADDI 2015 expands beyond the scope of the 2013 program to include lectures on drug development, including preclinical toxicity studies and clinical research. MCADDI 2015 also includes new lectures on phenotypic screening, antibody-drug conjugates, Pharmaceuticals and developability characteristics of drug candidates, and drug metabolism and pharmacokinetics.

MCADDI 2015 is designed for industrial scientists who are working in medicinal chemistry groups, biology, DMPK, toxicology and early clinical discovery teams, or are supporting drug discovery and development programs in collaboration with global pharmaceutical companies. MCADDI 2015 is also intended for academic scientists and postdoctoral fellows who are currently working in drug discovery, or who would like to become involved in teaching drug discovery and/or carrying out research in this area.

We hope that you will enjoy the course, and that what you learn this week will be of use to you in your career in drug discovery. We would greatly appreciate your feedback during the week and also on the evaluation form that will be provided. Your comments and ideas for improvement will help us improve the program in future years. We also ask for, and encourage, your participation in the discussions after the lecturers. Many of the faculty members will be present for most, or all, of the course for informal interactions.

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Advisory Board

Dr. Balu N. Balasubramanian, Pharma Innovation Sourcing Center, LLC

Dr. William Greenlee, MedChem Discovery Consulting, LLC

Prof. S. P. Thyagarajan, Sri Ramachandra University

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Sri Ramachandra University, Chennai, 2015

Acknowledgements

We would like to thank our Co-Sponsors:

American Chemical Society

IUPAC Division of Chemistry and Human Health

ACS Division of Medicinal Chemistry (MEDI)



**Division of
Medicinal
Chemistry**



We are also grateful to the following for generous financial support:

Lupin Pharma

Syngene

V ClinBio

Journal of Medicinal Chemistry

ACS Medicinal Chemistry Letters



Journal of
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ACS **Medicinal
Chemistry Letters**

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PROGRAM

Day 1: Sunday, February 8th, 2015

Venue: Lecture Hall V, 3rd Floor, Faculty of Dental Sciences

Discussion Leader – Dr. William Greenlee

2:30-3:15 PM	Registration Lecture Hall V, 3rd Floor, Faculty of Dental Sciences
3:15-3:30 PM	WELCOME Prof. S.P. Thyagarajan , Dean (Research), SRU Dr. Balu N. Balasubramanian , Pharma Innovation Sourcing Center LLC. USA
3:30-4:30 PM	<i>Lecture-1</i> “TARGET IDENTIFICATION AND VALIDATION” Dr. Manjunath Rama Rao , Bristol-Myers Squibb Biocon R &D Center, India
4:45-5:00 PM	<i>Tea break</i>
5:00-6:00 PM	<i>Lecture-2</i> “RECEPTORS, ENZYMES AND ION CHANNELS” Dr. Manjunath Rama Rao , Bristol-Myers Squibb Biocon R &D Center, India

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Day 2: Monday, February 9th, 2015

Venue: Seminar Hall & Lecture Hall IV, Medical College Building

Discussion Leader – Dr. Balu N. Balasubramanian

8:30-9:30 AM	<i>Lecture-3 Sponsored by the American Chemical Society</i> “BASIC PRINCIPLES OF MEDICINAL CHEMISTRY – 1” Prof. Thomas E Prisinzano, University of Kansas, USA
9:45-10:00 AM	<i>Coffee Break</i>
10:00-10:15 AM	WELCOME AND INTRODUCTION Prof. S.P. Thyagarajan, Dean (Research), SRU Dr. Balu N. Balasubramanian, Pharma Innovation Sourcing Center LLC. USA
10:15-10:30	INTRODUCTION OF PRESIDENT, AMERICAN CHEMICAL SOCIETY Dr. William Greenlee, Medchem Discovery Consulting, LLC, USA
	FELICITATION OF ACS PRESIDENT Dr. J.S.N. Murthy, Vice Chancellor, Sri Ramachandra University
10:30-11:00 AM	“THE AMERICAN CHEMICAL SOCIETY IN INDIA” Dr. Diane Schmidt, President, American Chemical Society Procter & Gamble, Inc., USA
11:00-11:15 AM	<i>Short Break</i>
11:15-12:15 PM	<i>Lecture-4 Sponsored by the American Chemical Society</i> “BASIC PRINCIPLES OF MEDICINAL CHEMISTRY – 2” Prof. Thomas E Prisinzano, University of Kansas, USA
12:15-1:30 PM	<i>Lunch Break</i>
1:30-2:30 PM	<i>Lecture-5 Sponsored by the American Chemical Society</i> “PHENOTYPIC SCREENING” Dr. Samitabh Chakraborti, Glenmark Pharma, India
2:45–3:45 PM	<i>Lecture-6 Sponsored by the American Chemical Society</i> “HIT-TO-LEAD PROCESS” Prof. Craig Lindsley, Vanderbilt University, USA
4:00-4:15 PM	<i>Tea break</i>
4:15-5:15 PM	<i>Lecture-7 Sponsored by the American Chemical Society</i> “LEAD OPTIMIZATION” Prof. Craig Lindsley, Vanderbilt University, USA

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Day 3: Tuesday, February 10th, 2015

Venue: Seminar Hall & Lecture Hall IV, Medical College Building

Discussion Leaders – Dr. Nick Meanwell, Dr. William Greenlee

8:30-9:30 AM	<i>Lecture-8</i> “STRUCTURE-BASED DRUG DESIGN” Dr. Vincent Stoll, AbbVie, USA
9:45-10:45 AM	<i>Lecture-9</i> “MOLECULAR MODELING” Dr. Vincent Stoll, AbbVie, USA
11:00-11:15 AM	<i>Tea Break</i>
11:15-12:15 PM	<i>Lecture- 10</i> “DRUG-LIKE PROPERTIES IN DRUG DISCOVERY” Dr. Swamy Yeleswaram, Incyte, USA
12:30-1:30 Noon	<i>Lunch Break</i>
1:30-2:30 PM	<i>Lecture-11</i> “PLASMA PROTEIN BINDING” Dr. Swamy Yeleswaram, Incyte, USA
2:45-3:45 PM	<i>Lecture-12</i> “G-PROTEIN COUPLED RECEPTORS” Prof. Craig Lindsley, Vanderbilt University, USA
3:45-4:00 PM	<i>Tea Break</i>
4:00-5:00 PM	<i>Lecture-13</i> “DRUG METABOLISM AND PHARMACOKINETICS” Dr. Swamy Yeleswaram, Incyte, USA

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Day 4: Wednesday, February 11th, 2015

Venue: Seminar Hall & Lecture Hall IV, Medical College Building

Discussion Leaders - Dr. Swamy Yeleswaran, Prof. Craig Lindsley

8:00-8:30 AM	<i>Group photo session</i>
8:30-9:30 AM	<i>Lecture-14</i> "BIOISOSTERES - 1" Dr. Nick Meanwell – Bristol-Myers Squibb, USA.
9:45-10:45 AM	<i>Lecture-15</i> "PHYSICOCHEMICAL PROPERTIES IN DRUG DESIGN" Dr. Nick Meanwell – Bristol-Myers Squibb, USA.
11:00-11:15 AM	<i>Tea Break</i>
11:15-12:15 PM	<i>Lecture-16</i> "PHARMACEUTICS AND DEVELOPABILITY CHARACTERISTICS OF DRUG CANDIDATES" Dr. Nancy Barbour, Bristol-Myers Squibb, USA.
12:30-2:00 PM	<i>Lecture-17 with working Lunch</i> <i>Sponsored by ACS Publications</i> "TOXIC PHARMACOPHORES" Dr. Nick Meanwell, Bristol-Myers Squibb, USA.
2:00-3:00PM	<i>Lecture-18</i> "PRECLINICAL TOXICITY EVALUATION - 1" Dr. Bruce Car, Bristol-Myers Squibb, USA.
3:15-4:15 PM	<i>Lecture-19</i> "PRECLINICAL TOXICITY EVALUATION - 2" Dr. Bruce Car, Bristol-Myers Squibb, USA.
4:30- 5:30 PM	Travel to Westin Hotel, Chennai

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Day 4: Wednesday, February 11th, 2015, 6:00 - 11:00 PM

Venue: Westin Hotels and Resorts, 154 Velachery Main Road, Chennai

Academia-Industry Round Table Discussion

Moderators – Dr. William Greenlee, Dr. Balu N. Balasubramanian

Time	Topic	Speaker
6:00 - 6:05 PM	Introduction and major questions for discussion	Dr. Balu N. Balasubramanian Pharma Innovation Sourcing Center LLC, USA, <i>and</i> Dr. William Greenlee Medchem Discovery Consulting LLC, USA
6:05 – 6:07 PM	Felicitation of ACS President and Experts	Shri. V.R. Venkataachalam Chancellor, Sri Ramachandra University
6:07 - 6:15 PM	What are the best ways for Government to encourage collaboration between academia and industry for drug discovery?	Dr. P.K. Sharma Director, Biotechnology Industry Research Assistance Council (BIRAC), Govt. of India, India
6:15 - 6:20 PM	What is the role of professional organizations like ACS in drug discovery education and industry-academia collaboration in the US and in India?	Dr. Diane Schmidt President, American Chemical Society, USA
6:20 - 6:25 PM	What is the landscape for collaboration between academia and industry in India?	Dr. Venkat Palle Senior Vice President, Discovery Research Lupin Pharma, India
6:25 - 6:35 PM	What are the most successful models of collaboration?	Dr. Joel Barrish Vice President Discovery Chemistry Bristol-Myers Squibb, USA <i>and</i> Professor Craig Lindsley Vanderbilt University, USA
6:35 - 6:40 PM	How can we advance the training of scientists in drug discovery in India?	Dr. S. P. Thyagarajan Professor Of Eminence and Dean of Research, Sri Ramachandra University, India
6:40 - 7:00 PM	Open Discussion	Participants and Panel
7:10 - 8:10 PM	Keynote Lecture by Dr. Joel Barrish, Bristol-Myers Squibb, USA <i>Sponsored by Lupin Pharmaceuticals</i>	
8:15 - 11:00 PM	Dinner Banquet	

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Day 5: Thursday, February 12th, 2015

Venue: Seminar Hall & Lecture Hall IV, Medical College Building

Discussion Leaders – Dr. Vincent Stoll, Prof. Thomas E Prisinzano

8:30-9:30 AM	Lecture-20 "CLINICAL DEVELOPMENT" Dr. Suresh Kankanwadi, Dr. Reddy Laboratories, India.
9:45-10:45 AM	Lecture-21 "INTRODUCTION TO BIOLOGICS" Dr. Nitin K Damle, Madronish Therapeutics, USA.
11:00-11:15 AM	<i>Tea Break</i>
11:15-12:15 PM	Lecture-22 "ANTIBODY DRUG CONJUGATES (ADCs)" Dr. Nitin K Damle, Madronish Therapeutics, USA.
12:30-1:30 PM	<i>Lunch Break</i>
1:30-2:30 PM	Lecture-23 "CASE HISTORY – 1, RUXOLITINIB, JAK2 INHIBITOR" Dr. Swamy Yeleswaran, Incyte, USA.
2:45-3:45 PM	Lecture-24 "CASE HISTORY – 2, SAROGLITAZAR, PPAR α/γ AGONIST" Dr. Mukul Jain, Zydus Cadila, India.
4:00-4:15 PM	<i>Tea Break</i>
4:15-5:15 PM	Lecture-25 "CASE HISTORY – 3, NCE DISCOVERY AND DEVELOPMENT FOR CHRONIC INFLAMMATORY DISEASES- FOUND IN TRANSLATION" Dr. Neelima Joshi, Glenmark, India.
5:30-6:00 PM	Concluding Remarks Dr. William Greenlee, Medchem Discovery Consulting LLC., USA Prof. S.P. Thyagarajan, Dean (Research), SRU, India.

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Dear MCADDI 2015 Participant:

As a scientist involved in drug research and development, you are well aware of the need for viewing your specific area of interest from an interdisciplinary perspective. To assist you, we cordially invite you to join the Division of Medicinal Chemistry of the American Chemical Society (ACS).

Each year the Division publishes a review of the previous year's literature in a volume entitled "Annual Reports in Medicinal Chemistry" in which all important aspects of the drug discovery process are covered. The chapters are compiled by chemists, pharmacologists, biochemists, microbiologists and others from industrial and academic settings. This annual volume is an excellent source of information for structures of novel medicinal agents, biological activity, and current concepts. The electronic version of **Annual Reports** is furnished to division members at no extra cost (publisher's price ca. ₹ 5200; \$85).

Stated below are the first year reduced Membership Dues applicable only for scientists who have participated in MCADDI 2015. We look forward to your participation in a large and stimulating scientific discipline.

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**APPLICATION FOR MEMBERSHIP, DIVISION OF MEDICINAL CHEMISTRY,
AMERICAN CHEMICAL SOCIETY**

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Mail to:

Dr. C. Vinodhini
Faculty of Pharmacy
Sri Ramachandra University
Porur, Chennai- 600116
vin_pharma@yahoo.com

Please send a check or money order payable to the Division of Medicinal Chemistry, ACS, or cash if you are submitting the application in person during the MCADDI 2015 Course.

If you prefer to use a credit card and pay in US dollars, please see the following page.

_____ Regular MCADDI 2015 Participant (₹ 920)

_____ Graduate or Postdoctoral Student Participant (₹ 495)

Name (Dr., Mr., Ms.) _____

Affiliation _____

Street _____

City _____

State/Union Territory _____

Signature _____

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