

Third Indo-US Lecture Series on Discrete Mathematical Chemistry: Special Lectures on Chemoinformatics & Bioinformatics

January 7–10, 2008

Bharathidasan University, Tiruchirappalli, Tamil Nadu, India

Computers are incredibly fast, accurate, and stupid. Human beings are incredibly slow, inaccurate, and brilliant. Together they are powerful beyond imagination.

—Albert Einstein

Chemoinformatics and bioinformatics can be looked upon as the two interconnected strands of a “double helix,” providing tools for modeling chemical interactions with biological systems, with both fields extensively employing mathematical concepts, information technology, and computational modeling. Many computational algorithms used in chemoinformatics and bioinformatics are based on discrete mathematics. The chemo-bio continuum is better understood through the mathematical analysis of problems. The Third Indo-US Lecture Series on Discrete Mathematical Chemistry will present a series of lectures and discussion forums aimed at educating present and future researchers working in the realms of the chemo- and bioinformatics.

continuity of such key ligand-biotarget interactions is critical for biological systems of widely varying complexity—from unicellular organisms to ecosystems—to function smoothly. Consequently, scientists need to understand and, if possible, quantitatively estimate the consequences of such ligand-receptor interactions for important cellular and metabolic processes. For example, a large number of drugs are small molecules that interact with specialized enzymes/receptors within specific biological compartments, thereby producing effects that bring a perturbed biological system back to homeostasis. Hence, it is necessary to use both chemical and biological knowledge pertaining to the drug or toxicant molecule and involved macromolecules, such as proteins, enzymes, and DNA sequences.

Lecture Series Focus

The Third Indo-US Lecture Series on Discrete Mathematical Chemistry will bring leading researchers from India and the United States together with young Indian students and scientists to discuss the fields of chemo- and bioinformatics, focusing on the following goals:

- Discuss mathematical & computational approaches to problems of chemistry & biology
- Introduce chemical modeling techniques including QSAR & QMSA, as well as other chemoinformatics approaches
- Introduce bioinformatics techniques applicable to genomics & proteomics
- Discuss the chemo-bio continuum & combined modeling strategies
- Provide a well-rounded introduction for graduate students & young research scientists
- Provide a forum for instruction & interaction between students/young scientists & established researchers

History of the Lecture Series

The Indo-US Lecture Series on Discrete Mathematical Chemistry evolved from the Indo-US Workshop Series on Mathematical Chemistry as a forum for introducing students to the fields of chemo- and bioinformatics.

<http://www.nrri.umn.edu/indousworkshop>

The concept of the Indo-US Workshop series was conceived by Subhash C. Basak, a Senior Scientist at NRRI, and received enthusiastic support from scientists in India and around the world.

This lecture series seeks to develop a forum where young scholars from abroad and India can interact with established scientists in the fields of mathematical chemistry and related disciplines and develop into productive researchers over time. The lecture series is a training program for scholars, rather than a forum for the presentation of scientific research.

The First Indo-US Lecture Series on Discrete Mathematical Chemistry was held in Bengalooru from January 8–11, 2007.

<http://www.nrri.umn.edu/indouslecture/2007>

Major sponsors of this event were the Department of Science and Technology (DST), New Delhi and the Indo-US Science and Technology Forum (IUSSTF), New Delhi.

Background

Most biological, pathological, toxicological, and biomedical processes are guided by small molecule interactions—such as endogenous receptor ligands, enzyme substrates and inhibitors related to metabolic pathways, and synthetic or natural modulators of critical biological systems. Maintaining the integrity and

The enthusiasm of the participants and presenters at this first lecture series ensured the continuation of the program, and the next event was held six months later. The second lecture series; organized jointly by Mary Matha Arts and Science College, Mananthavady, Kerala, India and NRRI/UMD, Duluth, USA; was held in Kalpetta from June 20–25, 2007. This event was sponsored by DST, NRRI, and the International Society of Mathematical Chemistry (ISMC).

<http://www.nrri.umn.edu/indouslecture/Kerala2007/>

The first two events covered a wide range of topics, from graph theory to specific applications of discrete mathematical chemistry to quantum chemistry. The third Indo-US lecture series will cover more specific areas, namely chemoinformatics and bioinformatics with an emphasis on applications. The Third Indo-US Lecture Series on Discrete Mathematical Chemistry: Special Lectures on Chemoinformatics and Bioinformatics, will be organized jointly by the Department of Bioinformatics, School of Life Sciences, Bharathidasan University, Trichy, India and NRRI/UMD, Duluth, Minnesota, USA at Tiruchirappalli from January 7–10, 2008.

How to Participate

Fifty outstanding participants will be selected from the departments of mathematics, physics, biophysics, chemistry, biochemistry, microbiology, biotechnology, bioinformatics, pharmaceutical chemistry, marine biology and statistics. Accommodation and food will be provided to all participants, and there is no registration fee. It is envisioned that the interaction between young researchers and resource persons will create a strong base for research in Discrete Mathematical Chemistry in India. Interested applicants should submit a completed copy of the registration form on or before **November 1, 2007** to:

Dr. S. Parthasarathy
Head of the Department
Department of Bioinformatics
Bharathidasan University
Tiruchirappalli 620 024, Tamil Nadu

Lecture Series Deadlines:

Nov. 1, 2007	Completed registration forms must reach Dr. Parthasarathy no later than November 1st, late forms will be discarded
Nov. 20, 2007	Notification of selected candidates
Jan. 7, 2008	Lecture Series begins at Bharathidasan University

Organized Jointly By:

Department of Bioinformatics
School of Life Sciences
Bharathidasan University
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Tamil Nadu, India



Natural Resources Research Institute
University of Minnesota Duluth
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NATURAL RESOURCES
RESEARCH INSTITUTE

List of Probable Resource Persons

BD Acharya, DST, New Delhi
 AS Nair, Univ of Kerala, India
 R Balakrishnan, SASTRA, Kumbakonam, India
 SC Basak, NRRI/UMD, Duluth, MN, USA
 A Bhattacharjee, Walter Reed Army Institute of Research, Silver Spring, MD, USA
 P Gautham, Anna Univ, Chennai, India
 S Gupta, Kolkata, India
 BD Gute, NRRI/UMD, Duluth, MN, USA
 VK Jayaram, NCL, Pune, India
 A Kulkarni, Accelrys Division of Pharmacoepia Inc., NJ, USA
 BK Mishra, Sambapalur Univ, India
 M Mumtaz, ATSDR/CDC, Atlanta, GA, USA
 A Nandy, Jadhavpur Univ, Kolkata, India
 R Natarajan, NRRI/UMD, Duluth, MN, USA
 GJ Niemi, NRRI/UMD, Duluth, MN, USA
 P Robinson, Henry M. Jackson Foundation, OH, USA
 V Subramanian, CLRI, Chennai, India
 P Venuvanalngam, Bharathidasan Univ, Trichy, India
 S Vishveshwara, IISc, Bengalooru, India

Please provide Xerox copies of the registration form to ensure that there are enough copies for interested students in your department. Each applicant must submit a separate registration form. Selected candidates will be notified by November 20, 2007.

Additional copies of the registration form can also be obtained from the lecture series website.