Department of Biotechnology
Ministry of Science and Technology
Government of India
DBT

National Institute of
Advanced Industrial Science
and Technology
AIST

DBT - AIST International Laboratory for Advanced Biomedicine

DAILAB

Classroom for Advanced & Frontier Education

CAFE

DAILAB-CAFE

Series - 13

Date and Time - March 03, 2016 (12:00~13:00)
Venue - Central 4 (5F) Room 5105

Speaker - Durai SUNDAR
Affiliation - Department of Biochemical Engineering and Biotechnology, DAILAB @ IIT Delhi, India
E-mail: sundar@dbeb.iitd.ac.in

Title : Structure-based drug design

Structure-based drug design (SBDD) is the design and optimization of a chemical structure with the goal of identifying a compound suitable for clinical testing – a drug candidate. It is based on knowledge of the drug's 3D-structure and how its shape and charge cause it to interact with its biological target, ultimately eliciting a medical effect. The effective implementation of lock and key concept proposed by Emil Fischer over a century ago is the key principle in SBDD, namely how precisely a drug interacts with its biological target. Experimentally two techniques, NMR spectroscopy in solution and X-ray crystallography of single crystals, are available to determine the bimolecular structure. In the absence of an experimentally characterized protein structure, a 3D model is designed using comparative protein modeling approaches. In cases where the primary structure is known, homology modeling utilizes the knowledge of the available experimental protein structures to design a 3D model for an unknown protein. Homology modeling approaches are well suited in cases where several reference structures are available, and in such cases one can go beyond the simple sequence similarities. Given a lead compound, an iterative process of designing improvements to the existing lead, synthesizing and testing the designed compounds, and solving the 3D structure of each improved compound with the target, usually begins. Receptor-based approaches include *de novo* design and molecular docking. Theoretical and computational methods employed in docking are molecular dynamics, Monte Carlo, Genetic algorithms, fragment-based, Point complementary & Distance geometry methods. In this seminar, I will give an overview of the SBDD pipeline along with details of docking approaches in computational biology and drug design. Representative examples will be taken to illustrate different approaches.

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SERIES - 13

Speaker: Dr. Durai SUNDAR
Topic: *Structure Based Drug Design*
Date: 3rd March 2016 (1500-1600 hours JST)
Host: AIST, Japan

Dear Dr Sundar
Thanks for Mentoring CAFÉ Series 13
We all highly appreciate your time and efforts !
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IIT-Delhi, India

Hanyang University, South Korea

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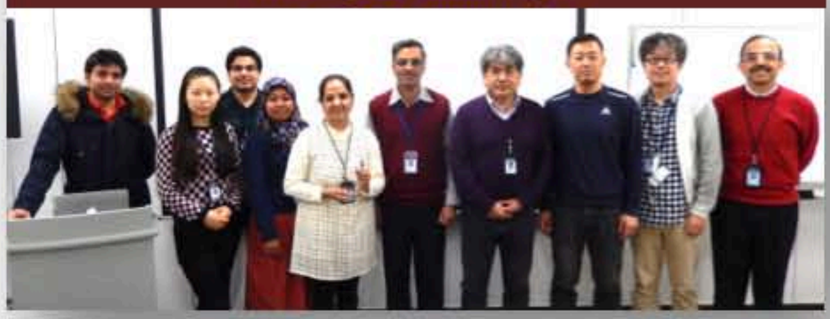

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