



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**

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# 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

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## 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: 3<sup>rd</sup> 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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