

**Indian Council of Medical Research (ICMR), Council of Scientific and Industrial
Research (CSIR) and JSS University, Mysore**

Co-Sponsored

Two days National Workshop on

**“Computational Tools for Protein Modeling and Lead Optimization in Drug
Discovery”**

Date: 7th and 8th March, 2014

Organized by:

Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty

A Brief Report

Two Days National Workshop on “Computational Tools for Protein Modeling and Lead Optimization in Drug Discovery” was conducted on 7th and 8th of March, 2014. The venue of workshop was seminar Hall of J. S. S. College of Pharmacy, Ooty. On 7th of March 2014 after breakfast (8.30-9.00 AM) registration of delegates started at 9.00 AM. After describing the importance of computer aided drug design in modern day to day research Dr. Md. Afzal Azam delivered the welcome address and requested distinguished speakers to release the workshop chronicle. Dr. S.P. Dhanabal, Principal, J. S. S. College of Pharmacy, Ooty and Chairman of the Workshop also highlighted the importance of “Computational Tools for Protein Modeling and Lead Optimization in Drug Discovery” process. Dr. K. Elango, Senior Professor, Department of Pharmacology also highlighted the importance of “Computational Tools for Protein Modeling and Lead Optimization in Drug Discovery” process.

Distinguish speakers present for the two days National workshop:

1. Dr. K. Raghu, Vice President, Schrodinger Inc., Bangalore.
2. Dr. S. P. Muthukumar, Principal Scientist, Biochemistry and Nutrition Department, CSIR-Central Food Technological Research Institute (CFTRI), Mysore
3. Dr. M. Ravi Kumar, Senior Scientist Applications, Schrodinger Inc., Bangalore.
4. Dr. R. S. Rathore, Senior Scientist Applications, Schrodinger Inc., Bangalore.
5. Dr. Md. Afzal Azam, Professor and head, Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty.

On the first day of workshop i.e. on 7th of March two presentations and hands-on-training sessions were organized on Ligand based drug design covering Pharmacophore modeling,

substructure matching, 2D and 3D QSAR. For hands-on-training delegates, our faculty, research scholars and PG students were provided with laptops by Schrodinger Inc., USA.

Second day of workshop i.e. on 8th of March started at 9.30 AM and two presentations and hands-on-training sessions were organized on Structure based drug design covering ligand preparation, protein modeling, homology modeling, different docking tools and methods, interpretation of docking results and fragment based drug design. For hands-on-training delegates, our faculty, research scholars and PG students were provided with laptops by Schrodinger Inc., USA.

A total of 40 delegates from various parts of country were selected for this workshop including senior faculty, research scholars and PG students from various discipline like Bioinformatic, Biotechnology, Pharmacology and Pharmaceutical Chemistry specialization.

Certificates are also issued to all delegates. and eminent resource persons. Honorarium and certificates were also issued to all speakers by dignitaries. Dr. R. Kalirajan, Organizing Secretary of workshop conveyed the vote of thanks at the end of valedictory function.

Herewith we take this opportunity to thank you for giving us opportunity to organize the workshop.

Herewith we are submitting the report on workshop.

Thanking You

1. **Dr. Md. Afzal Azam** (Convenor)

2. **Dr. R. Kalirajan** (Organizing secretary)

Inauguration



Chronicle Release



Hands on Training by scientists from Schrodinger LLC



Group Photos with Speakers & Delegates

