

**DST-SERB, New Delhi and JSS University, Mysuru**

Co-Sponsored Two days National Seminar on

**“Recent Advances in Drug Design using Computational Chemistry Tools- Case Study”**

**Date(s): 4<sup>th</sup> and 5<sup>th</sup> November, 2016**

**Organized by:**

**Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty**

**A Brief Report**

Two Days National Seminar on “**Recent Advances in Drug Design using Computational Chemistry Tools- Case Study**” was conducted on 4<sup>th</sup> and 5<sup>th</sup> of November, 2016 at the auditorium of JSS College of Pharmacy, Ooty. On 4<sup>th</sup> of November 2016 after breakfast (8.30-9.00 AM) registration of delegates started at 9.00 AM. The Kit bags and other seminar materials are issued to all the delegates.

After describing the importance of computational chemistry tools in modern day to day research **Dr. Md. Afzal Azam** delivered the welcome address. The seminar was inaugurated by all the dignitaries by lighting the lamp and the seminar chronicle in the CD format was released by the distinguished speakers. **Dr. K. Elango**, Senior Professor, Department of Pharmacology also highlighted the importance of “Computational Tools for in Drug Discovery” process.

Distinguish speakers present for the two days National seminar:

1. **Dr. M. Karthikeyan**, Principal Scientist ,CSIR-National chemistry laboratory, pune
2. **Dr. Pritesh Bhat**, Senior Scientist Applications, Schrodinger Inc., Bangalore.
3. **Mr. Vinod D**, Scientist Applications, Schrodinger Inc., Bangalore.

On the first day of seminar i.e. on 4<sup>th</sup> of November the presentation on the topic "Chemoinformatics for Drug Discovery: Recent Advances" was given by **Dr. M. Karthikeyan**. Then presentations and hands-on-training sessions are given by **Dr. Pritesh Bhat** and **Mr. Vinod D** from Schrodinger Inc., Bangalore, on Ligand based drug design covering Pharmacophore modeling, substructure matching,

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

Second day of workshop i.e. on 5<sup>th</sup> of November started at 9.00 AM and two presentations and hands-on-training sessions are given by **Dr. Pritesh Bhat** and **Mr. Vinod D** from Schrodinger Inc., Bangalore, 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.

In the afternoon session, nearly 15 oral presentations were delivered by the delegates in various topics and the best oral presentation award was given.

A total of 85 delegates from various parts of country were selected for this seminar including senior faculty, research scholars and PG students from various discipline like Bioinformatics, 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 seminar.

The seminar was published in daily news papers like, Dhinamani, Dhinaboomi, Dhinamalar, Dhinakaran, Makkal Kural, Tamil sudar and The Trinity mirror.

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

