

One day webinar on
**Recent Advance in Drug Design: State of the Art Tools for Drug Design and Drug
Discovery**
scheduled on **23rd June 2020**

Organized by
**Pharmacy Education Unit, Department of Pharmaceutical Chemistry,
JSS College of Pharmacy, Ooty**
In Association with **Schrodinger, Bangalore, India**

A Brief Report

One Day webinar on "**Recent Advance in Drug Design: State of the Art Tools for Drug Design and Drug Discovery**" was conducted on **23rd June 2020** by JSS College of Pharmacy, Ooty in association with Schrodinger LLC, Bengaluru.

The workshop was inaugurated by **Dr. S. P. Dhanabal**, Principal, JSSCP, Ooty and patron of webinar. **Dr. S. Ponnusankar**, Professor and Co-convenor delivered the welcome address. **Dr. Md. Afzal Azam**, Professor & Head and Convenor highlighted the importance of computational chemistry tools in modern day to day research and genesis of the workshop. **Dr. R. Raghu**, Vice President, Schrodinger LLC, Bengaluru briefed about the importance of computational tools in the modern drug discovery.

Earlier, prior to the first session at 11:00 AM, **Dr. R. Kalirajan**, Organizing Secretary introduced the first speaker **Dr. Pritesh Bhat**, Senior Scientist - Applications, Schrodinger LLC., Bengaluru and followed by the presentation on "**Recent Advance in Drug Design**" covering ligand preparation, protein modeling, homology modeling, different docking tools and methods, interpretation of docking results was delivered.

At 12.15 pm, the next speaker **Dr. Prajwal Nandekar** Senior Scientist - Applications, Schrodinger LLC., Bengaluru was introduced by **Dr. S. Jubie**, Asst. Prof, Dept. of Pharm Chemistry and followed the presentation on topic "Molecular Dynamics Simulation: Applications in Drug Discovery" was delivered.

After lunch break, the next presentations at 2.30 pm was given by **Dr. Pritesh Bhat**, Senior Scientist - Applications, Schrodinger LLC., Bengaluru, on topic “**Advanced Drug Design Tools – WaterMap, FEP+ And Machine Learning Tools**”.

At 3.30 pm the last speaker of the webinar **Mr. Vinod Devaraji**, Senior Scientist, Schrödinger LLC, Bengaluru was introduced by **Dr. B. Gowramma**, Asst. Prof, Dept. of Pharm Chemistry, and presentation on topic “**Ligand Based Drug Design Approaches - Pharmacophore, 3D-QSAR, Auto QSAR**” was delivered the session was continued up to 4.30 pm.

After the completion of each session, **Ms. Shelvia Malik**, Accounts Manager and Business Development Officer, Schrodinger LLC, Bangalore coordinated about the Question and Answer session and clarified the queries asked by the delegates.

A total of 2128 delegates have registered from various countries such as India, United States of America, Saudi Arabia, Bahrain, Hong Kong etc. More than 50% of delegates are senior faculty, and research scholars from various discipline like Bioinformatics, Biotechnology, Pharmacology and Pharmaceutical Chemistry.

Dr. Gomathi Subramanian, Asst. Professor, Dept. of Pharm Chemistry, proposed the vote of thanks.

Herewith we take this opportunity to thank, JSS AHER, Mysuru and especially Dr. Ravindra and his team for their IT support for the smooth conduct of this webinar through ZOOM and Mr. C. Jayakumar, Asst. prof and Mr. Gautham, from JSSCP, Ooty for their technical support to organize the webinar successfully..

Thanking You

1. **Dr. Md. Afzal Azam** (Convenor)
2. **Dr. R. Kalirajan** (Organizing secretary)

Some Photos of webinar

Presentation by Dr. Pritesh Bhat from Schrodinger LLC

LIVE on YouTube | You are viewing Dr. Pritesh Bhat's screen | View Options

Required Inputs for Protein-Ligand Docking – Ligands (LigPrep)

- Glide will only dock ligand states that are provided
- Recommendations for prepared ligand structures
 - Use LigPrep to generate low energy ionization/tautomeric states for ligands
 - Epik state penalties that estimate free energy required to generate ionization state in water with corrections for interaction with metal sites
 - Typical expansion of compounds by ionization/tautomeric/stereo expansion is 2.5x
 - Increase or decrease pH value and +/- range depending on target physiological location and project goals

State penalty=0.0 kcal/mol

State penalty=1.43 kcal/mol

Methotrexate bound to DHFR (1U72)

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Presentation by Dr. Prajwal Nandekar from Schrodinger LLC

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Crystal structures are a picture while MD simulations are a movie

Statics crystal structure | MD simulation

The image shows three protein-ligand complexes. On the left, a 'Statics crystal structure' is shown as a multi-colored ribbon model of a protein with a purple ligand. In the middle, a grey surface representation of the protein with the purple ligand. On the right, an 'MD simulation' is shown as a grey surface representation of the protein with an orange ligand, illustrating conformational changes. A red dot is visible at the bottom right of the MD simulation.

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Presentation by Mr. Vinod Devaraji from Schrodinger LLC

Understanding Pharmacophore:

What functional features do they have in common?

ADHN features

- Negative Ionizable
- H-Bond Donor
- Aromatic
- Hydrophobic

- Generate conformers

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Mr. Vinod Devar...

Chat Raise Hand Q&A Leave

At JSSCP, Ooty

