

# Introduction to Computational Drug Design

*Co-Organised by Schrödinger and Pharmacy Council of India*

*Theory - Demo - Hands-on*

## Inauguration

**Date: 21<sup>st</sup> Sep 2020 ~ Time: 10 AM**

**Prof. B Suresh, President, Pharmacy Council of India**

Computational molecular modeling tools are changing the world of drug design and formulation development. The online “Introduction to Computational Drug Design” webinar series will demonstrate how industry-leading computational molecular modeling tools are used to aid in drug design and formulation development; and to incorporate these tools into your curriculum and research projects.

This will be an exceptional value addition to your professional development in the form of new skill enhancement. The online webinar series will provide basic theoretical and practical applications of computational modeling using active learning strategies.

The programme is broken into three phases:

- I. Lectures concentrated on the theory and basics
- II. Demonstration of Schrödinger modeling tools
- III. Hands-on experience with the Schrödinger software

**Eligible Participants:** Undergraduates (3rd and Final Year Students); Post Graduates; Research Scholars; Faculty Members/Academicians

Register at <https://www.schrodinger.com/ddcourse>

If you have any questions, please email [shelvia.malik@schrodinger.com](mailto:shelvia.malik@schrodinger.com)

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## Agenda

**Phase I:** Lectures on theory and basics of modeling

**Frequency:** 1-hour sessions 22<sup>nd</sup> to 1<sup>st</sup> Oct at 10.00 - 11.00 AM & 11.15 AM - 12.15 PM

**Presenters:** Speakers from Schrödinger EU, Schrödinger India, Glenmark, and Syngene

### Topics:

- Introduction to computer-aided drug design - 22<sup>nd</sup> Sep
- Target structure understanding - 22<sup>nd</sup> Sep
- Ligand library for simulation - 23<sup>rd</sup> Sep
- Preparing protein and ligand for simulation - 23<sup>rd</sup> Sep
- Identifying ligand binding site - 24<sup>th</sup> Sep
- Theory, principles, methods of molecular docking - 24<sup>th</sup> Sep
- Virtual screening to prioritizing the molecules - 25<sup>th</sup> Sep
- Need for flexible docking and covalent docking - 25<sup>th</sup> Sep
- Molecular dynamics simulations theory and analysis - 28<sup>th</sup> Sep
- When the target protein structure is not there? - 28<sup>th</sup> Sep
- Ligand-based drug design: QSAR approach - 29<sup>th</sup> Sep
- Pharmacophore modeling - 29<sup>th</sup> Sep
- Quantum Mechanics for drug design - 30<sup>th</sup> Sep
- Computational biologics design - 30<sup>th</sup> Sep
- Computational formulation design - 1<sup>st</sup> Oct

Additional industrial partners presentation on case studies (10.30 AM - 12.30 PM)

- Syngene - 3<sup>rd</sup> Oct
- Glenmark - 16<sup>th</sup> Oct

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## Phase II: Demonstration of Schrödinger modeling tools

**Frequency:** Daily sessions 5<sup>th</sup> Oct to 23<sup>rd</sup> Oct from 10.00 - 11.00 AM

### Hands-on Demo Sessions:

- Maestro GUI: Sketching, molecular visualization, build/edit molecule - 5<sup>th</sup> Oct
- Protein preparation and ligand preparation - 6<sup>th</sup> Oct
- Binding site identification - 7<sup>th</sup> Oct
- Molecular docking methods and analysis of docking - 8<sup>th</sup> Oct
- Induced-fit docking (IFD) and covalent docking (CovDock) - 9<sup>th</sup> Oct
- Homology modeling and loop refinement; structure validation - 12<sup>th</sup> Oct
- Pharmacophore modeling and screening large compound libraries (from multiple ligands, single ligand, apo-protein, protein-ligand complex, and protein-protein interface) - 13<sup>th</sup> Oct
- Combine modeling and experimental data for atom/field QSAR development: 3D atom-based QSAR, activity prediction - 14<sup>th</sup> Oct
- 1D/2D QSAR model building; AutoQSAR - 15<sup>th</sup> Oct
- De novo molecular design: Reaction-based enumeration, combinatorial library design, biosteric modification, Ligand Designer, etc. - 16<sup>th</sup> Oct
- Molecular dynamics simulations and trajectory analysis: System preparation, simulation, analysis, simulation interaction diagram - 19<sup>th</sup> Oct
- Biologics development: Antibody design; protein-protein interaction analysis - 20<sup>th</sup> Oct
- Protein liability and protein engineering tools: Protein aggregation prediction with AggScore, protein hotspot analysis, residues mutations, residue-scanning, cysteine scanning, and affinity maturation - 21<sup>st</sup> Oct
- Quantum mechanics (QM) in drug design: Geometry optimization, spectra predictions, QM-MM calculations - 22<sup>nd</sup> Oct
- Computer-aided formulation design and analysis - 23<sup>rd</sup> Oct

**Phase III:** The qualified participants will have the opportunity to install the software locally on your computers and utilize the tools to take up a case study. Technical and scientific support will be provided by Schrödinger.



# Syngene

Putting Science to Work

Register at <https://www.schrodinger.com/ddcourse>

If you have any questions, please email [shelvia.malik@schrodinger.com](mailto:shelvia.malik@schrodinger.com)