SCHRÖDINGER®

Introduction to Computational Drug Design

Co-Organised by Schrödinger and Pharmacy Council of India

Theory - Demo - Hands-on

Inauguration

Date: 21st 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

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Agenda

Phase I: Lectures on theory and basics of modeling

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

Additional industrial partners presentation on case studies (10.30 AM - 12.30 PM)
- Syngene - *3rd Oct*
- Glenmark - *16th Oct*

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Phase II: Demonstration of Schrödinger modeling tools

Frequency: Daily sessions 5th Oct to 23rd Oct from 10.00 - 11.00 AM

Hands-on Demo Sessions:

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

Glenmark — A new way for a new world

JSS ACADEMY OF HIGHER EDUCATION & RESEARCH (DEEMED TO BE UNIVERSITY) MYSURU

MANIPAL ACADEMY of HIGHER EDUCATION (Deemed to be University under Section 3 of the UGC Act, 1956)

Syngene — Putting Science to Work

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