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

K. K. WAGH COLLEGE OF PHARMACY
(B. Pharmacy & D. Pharmacy)
Hirabai Haridas Vidyanagari, Amrutdham, Panchavati, Nashik - 422 003. (Maharashtra) India.
☎: 0253 - 2221121, 2517003, 2510262 Web : www.pharmacy.kkwagh.edu.in
Email: principal-bpharmacy@kkwagh.edu.in, disp-bpharmacy@kkwagh.edu.in
(Affiliated to Dr. Babasaheb Ambedkar Technological University, Lonere, MSBTE, Mumbai & Approved by PCI)

Course G - Syllabus with course outcomes

Title of course: Introduction to Computational Drug Design

Duration: 2020-21 (21/09/2020 to 23/10/2020) [one month (online)]

Course Coordinator: Schrödinger and PCI

SYLLABUS

- Introduction to computer-aided drug design
- Target structure understanding
- Ligand library for simulation
- Preparing protein and ligand for simulation
- Identifying ligand binding site
- Theory, principles, methods of molecular docking
- Virtual screening to prioritizing the molecules
- Need for flexible docking and covalent docking
- Molecular dynamics simulations theory and analysis
- When the target protein structure is not there?
- Ligand-based drug design: QSAR approach
- Pharmacophore modeling
- Quantum Mechanics for drug design
- Computational biologics design and formulation design
- Demonstration of Schrödinger modeling tools
- Hands-on experience with the Schrödinger software

COURSE OUTCOMES

The course is value addition to professional development in the form that

- demonstrate how industry-leading computational molecular modeling tools are used to aid in drug design and formulation development
- incorporate these tools into curriculum and research projects
- provide basic theoretical and practical applications of computational modeling using active learning strategies

K. K. WAGH COLLEGE OF PHARMACY NASHIK-3

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List of students

Title: Introduction to Computational Drug Design

Sr. No	Name of Student
1.	Janhavi Dilip Borse
2.	Ashwini Anna Parekar
3.	Bichave Mugdha Sandeep
4.	Patil Aishwarya Vasantrao
5.	Yogita Ashok Khairnar
6.	Rishabh Gopal Chandak
7.	Shaikh Sadaf Qadir
8.	Pratiksha Vasant Jadhav

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Attendance Sheet

Introduction to Computational Drug Design

(21/09/2020 to 23/10/2020) (online)

Sr. No	Name of Student	Signature
1.	Janhavi Dilip Borse	Jorase
2.	Ashwini Anna Parekar	AParekar
3.	Bichave Mugdha Sandeep	Bichave
4.	Patil Aishwarya Vasantrao	Apatil
5.	Yogita Ashok Khairnar	Kogita
6.	Rishabh Gopal Chandak	RChandak
7.	Shaikh Sadaf Qadir	
8.	Pratiksha Vasant Jadhav	PJadhav

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Panchavati, Nashik-422 003.

Course completion certificate

SCHRÖDINGER. JSS ACADEMY OF HIGHER EDUCATION & RESEARCH MYSURU MANIPAL ACADEMY of HIGHER EDUCATION

Introduction to Computational Drug Design

(Theory - Demo - Hands-on)

This is to certify that

Janhavi Dilip Borse

has participated and Qualified in the Assessment Test in the above program

Co-Organized by
Schrödinger & Pharmacy Council of India
between 21st Sep - 23rd Oct 2020.

Dr B. Suresh	Dr R. Raghu	Dr S. P. Dhanabal	Dr C. Mallikarjuna Rao
President	Vice President	Principal	Principal
Pharmacy Council of India	Schrödinger	JSS College of Pharmacy, Ooty	Manipal College of Pharmaceutical Sciences, Manipal

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This is to certify that

Ashwini Anna Parekar

has participated and Qualified in the Assessment Test in the above program

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Bichave Mugdha Sandeep

has participated and Qualified in the Assessment Test in the above program

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Patil Aishwarya Vasantrao

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Yogita Ashok Khairnar

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Rushab Gopal Chandak

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Shaikh Sadaf Qadir

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Pratiksha Vasant Jadhav

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