

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.

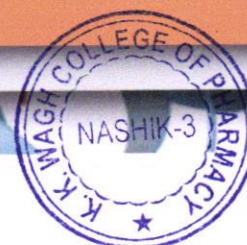
The programme is broken into three phases:

- 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 shelviamalik@schrodinger.com





K. K. WAGH COLLEGE OF PHARMACY

(B. Pharmacy & D. Pharmacy)

Hirabai Haridas Vidyanagari, Amrutdham, Panchavati, Nashik - 422 003. (Maharashtra) India.

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(Affiliated to Dr. Babasaheb Ambedkar Technological University, Lonere, MSBTE, Mumbai & Approved by PCI)

Title of course: Introduction to Computational Drug Design

Course G - Syllabus with course outcomes

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



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List of students

Course G - 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 Vasant
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	
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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K. K. Wagh College of Pharmacy
Panchavati, Nashik-422 003.

Vision: To develop the institute as a global brand, imparting quality education in the pharmacy field, thereby, creating competent and expert pharmacists ready to serve the healthcare industry and society.

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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
President
Pharmacy Council
of India

Dr R. Raghu
Vice President
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Principal
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Dr C. Mallikarjuna Rao
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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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Bichare Mugdha Sandeep

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This is to certify that
Patil Ashwarya Vasantrao

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Yegita Ashok Khairnar

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Rushab Jugal Chandak

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Shaikh Sadaf Qadir

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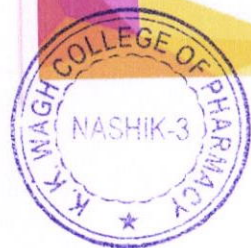
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Pratiksha Vasant Jadhav

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