KLE College of Pharmacy, Bengaluru

A Constituent Unit Of KLE Academy Of Higher Education And Research, Belagavi

Value Added Course on In-Silico Drug Design

Offered By-

Department of Pharmaceutical Chemistry

KLE College of Pharmacy, Bengaluru

2nd Block Rajaji Nagar, Bengaluru (080 2332 4529)

Value Added Course on

IN-SILICO DRUG DESIGN

Preamble

In the dynamic landscape of modern medicine and pharmaceutical research, the emergence of in-silico drug design stands as a pivotal and transformative discipline. This rapidly evolving field harnesses the power of computational tools and cutting-edge technologies to revolutionize the way we discover, design, and develop pharmaceutical compounds.

The In-Silico Drug Design Value-Added Course is designed to be a beacon of knowledge and innovation in this exciting domain. Rooted in the fusion of computational science, biology, chemistry, and healthcare, this course aims to equip learners with the skills and insights needed to navigate the complexities of drug discovery in the digital age.

As we embark on this educational journey, we recognize the pressing need to address the challenges of our time. The rising demand for novel therapeutics, the imperative of personalized medicine, and the quest for faster and more cost-effective drug development solutions are driving the importance of in-silico drug design to unprecedented heights. This course seeks to bridge the gap between theory and practice, empowering participants to contribute to groundbreaking advancements in drug discovery.

Our commitment to excellence is underpinned by several key principles:

1. **Interdisciplinary Expertise**: We believe that the intersection of diverse disciplines is where innovation thrives. Our course draws from the expertise of computational scientists, biologists, chemists, and pharmaceutical professionals to provide a holistic learning experience.
2. **Cutting-Edge Technology**: In the era of artificial intelligence, machine learning, and high-performance computing, we are dedicated to delivering hands-on training that leverages the latest tools and techniques. Participants will gain proficiency in state-of-the-art software and methodologies.
3. **Ethical and Responsible Practice**: We emphasize the importance of ethical considerations in drug design. Our curriculum addresses the ethical and regulatory challenges associated with in-silico drug discovery to ensure that learners develop a strong sense of responsibility in their research and development endeavors.

4. **Collaboration and Networking**: In the spirit of open science, we encourage collaboration and knowledge-sharing among participants. Our course fosters a supportive community where learners can exchange ideas, collaborate on projects, and build lasting professional networks.
5. **Real-World Applications**: Practicality is at the heart of our course. Through case studies, hands-on exercises, and industry insights, participants will gain the practical skills and knowledge necessary to make a meaningful impact in the field.

The In-Silico Drug Design Value-Added Course is not just an educational endeavor but a journey of exploration and innovation. We invite learners from diverse backgrounds who are passionate about transforming the future of healthcare through computational drug discovery. Together, we aim to unlock the full potential of in-silico drug design and usher in a new era of precision medicine, where groundbreaking therapeutics are just a click away.

Scope

The scope of an in-silico drug design value-added course is broad and holds significant relevance in the fields of pharmaceutical research, healthcare, and biotechnology. Such a course can provide participants with valuable skills and knowledge that can be applied in various professional settings like Pharmaceutical research and Development, Bioinformatics and Computational Biology, Data Science and AI in Healthcare etc.

Objectives

The objectives of an in-silico drug design value-added course are

- To provide participants with a comprehensive understanding of the principles, techniques, and practical applications of in-silico drug design.
- To equip learners with the knowledge and skills necessary to contribute effectively to drug discovery and development using computational methods.

Outcomes

Upon the completion of course students shall able to:

1. Explain the process of drug discovery and drug design.
2. Discuss about various approaches used in Insilico drug designing.
3. Describe the role of molecular docking, virtual screening, Pharmacophore mapping and Homology modeling in drug discovery and development.
4. Discuss and able to handle various software, servers and databases used in drug design.
5. Understand the Real-world applications and challenges faced in drug discovery process by industry experts or academicians.

Future Prospects and Job Opportunities

- ✓ Drug Discovery Research
- ✓ Computational Chemistry
- ✓ Bioinformatician
- ✓ Data Scientist in Healthcare

Course Content 30 Hours

MODULE NO.	TITLE OF THE MODULE	DURATION (HOURS)
I	**Introduction to In-Silico Drug Design**	6
II	**Molecular Docking**	6
III	**Pharmacophore Mapping**	6
IV	**Hands on Training on Software**	6
V	**Industry Insights and Guest Lectures**	6

Modules Wise Content

Module-I	In-Silico Drug Design	6 Hours
1	Overview of Drug Discovery and Development Process	1 Hour
2	Approaches of Drug Design	1 Hour
3	Types of in-silico methods: Molecular docking, Virtual screening, Pharmacophore mapping, QSAR ADMET prediction, Homology modeling.	1 Hour
4	Network Pharmacology: Overview	1 Hour
5	Software tools and databases used in silico drug design	1 Hour
6	Future of in-silico Drug design- Introduction to Artificial intelligence and Machine learning	1 Hour

Module Outcomes:

Upon the completion of this module students will be able to:

1. Explain the basic concepts of Drug Discovery and Drug Design.
2. Discuss about virtual screening techniques and network pharmacology.
3. Discuss about Artificial Intelligence and Machine Learning

Module II	Molecular Docking	6 Hours
7	Introduction	1 Hour
8	Molecular Docking approaches	1 Hour
9	Target Identification and Target preparation	1 Hour
10	Ligand Preparation	1 Hour
11	Molecular Docking Process, Result Analysis and Prediction of Binding site	1 Hour
12	Virtual screening methodologies using Docking approach	1 Hour

Module Outcomes: Upon completion of this module the students will be able to:

1. Describe the approaches of molecular docking.
2. Outline the steps involved in molecular docking.
3. Identify drug like candidates by performing molecular docking.

Module III	Pharmacophore Mapping	6 Hours
13	Definition and significance of Pharmacophores	1 Hour
14	Role of Pharmacophores in drug design	1 Hour
15	Types of Pharmacophore features (e.g., hydrogen bond donors/acceptors, aromatic rings)	1 Hour
16	Pharmacophore hypothesis generation	1 Hour
17	Validation and refinement of pharmacophore models	1 Hour
18	Virtual screening methodologies using Pharmacophore models	1 Hour

Module Outcomes: Upon completion of this module the students will be able to:

1. Describe the approaches of Pharmacophore mapping.
2. Outline the steps involved in Pharmacophore mapping.
3. Identify drug like candidates by performing Pharmacophore based virtual Screening.

Module-IV	Hands on Training on Softwares	6 Hours
19	Drawing chemical Structures(Chemdraw/Chemsketch) and retrieval 3D structure of Protein from Protein databank and its analysis	1 Hour
20	Drug Likeness, ADME and bioavailability Screening(Molsoft/Swiss ADME)	1 Hour
21	Insilico toxicity prediction(Protox-II)	1 Hour
22	Pharmacophore mapping(Ligandscout/ Pharmamapper)	1 Hour
23	Homology modeling(Modeller)	1 Hour
24	Molecular Docking and Results analysis (Molegro/CB dock/Swiss Dock etc.) and virtual screening(VSTH server/drug like server)	1 Hour

Module Outcomes: Upon completion of this module students will be able to:

1. Handle basic and advanced tools of Drug Design.
2. Evaluate drug like molecules on the basis of their physicochemical, pharmacokinetic properties, toxicity and binding interactions.

Module-V	Industry Insights and Guest Lectures	6 Hours
25	Invited talks by experts from pharmaceutical industry and academia	2 Hour
26	Real-world applications and challenges faced in drug discovery	2 Hour
27	Interactive sessions with professionals involved in computational drug design	2 Hour

Module Outcomes: Upon completion of this module the students will be able to:

1. List out real-world applications and challenges faced in drug discovery.
2. Exposure to practical in-silico drug design methods and tools.

Reference Books:

1. Smith HJ, Williams H, eds, "Introduction to the principles of Drug Design" Wright Boston.
2. Silverman R.B. "The organic Chemistry of Drug Design and Drug Action" Academic Press New York.
3. Robert GCK, ed., "Drug Action at the Molecular Level" University Prak Press Baltimore
4. Martin YC. "Quantitative Drug Design" Dekker, New York.
5. Delgado JN, Remers WA eds "Wilson & Gisvolds's Text Book of Organic Medicinal & Pharmaceutical Chemistry" Lippincott, New York.
6. Foye WO "Principles of Medicinal chemistry 'Lea & Febiger.
7. Koro lkovas A, Burckhalter JH. "Essentials of Medicinal Chemistry" Wiley Interscience.
8. Wolf ME, ed "The Basis of Medicinal Chemistry, Burger's Medicinal Chemistry" John Wiley & Sons, New York.
9. Patrick Graham, L., An Introduction to Medicinal Chemistry, Oxford University Press.

Eligibility: B. Pharm (III & IV Year) and PG Students

Duration: 30 Hours

Added Benefits for the Participating Students:

- Hands on training
- Certificate of course completion
- Exposure to computational chemistry labs
- Post training
- Assistance to conduct project work related to course

Course Coordinator:

Dr. Priyanka Kamaria
Assistant Professor, Department of Pharmaceutical Chemistry
KLE College of Pharmacy, Bangalore

Contact Details:

Dr. S. S. Karki
HOD, Department of Pharmaceutical Chemistry
KLE College of Pharmacy, Bangalore
Contact No.- 9448017123
E mail id- subhasskarki@gmail.com

Dr. Rajamma AJ
Principal
KLE College of Pharmacy, Bangalore
Contact No.- 9731016717
E mail id-
abburjayaramu6@gmail.com