



Value Added Course on

Computational Tools in Drug Design

Offered by

Dept. of Pharmaceutical Chemistry

KLE COLLEGE OF PHARMACY

Belagavi

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Our B. Pharm Program has been accredited by NBA for a period of 6 years (from July 2019 to June 2025)



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Preamble

Drug Discovery is a process which aims to identify pharmacologically active lead from set of compounds. It is expensive and time-consuming process involves many phases. Drug Design is a technique of lead modification and it is very important stage in drug development process to yield a desired drug candidate with improved pharmacokinetic and pharmacodynamic effect. At present a new approach is being tried to investigate a drug candidate using modern discovery tools on the basis of target structure. The advanced technologies and tools employed in drug discovery and drug design processes involves computational tools, combinatorial chemistry, genomics, proteomics, bioinformatics, and chemoinformatics and many other techniques.

Computational tools involve the use of various softwares, servers, informatics and databases which are useful in order to investigate physicochemical and pharmacokinetic properties of molecules. These tools are also useful in order to predict how a lead molecule or optimized lead can interact with a specific target. The results of computational screening give valuable information about several properties of drug candidate like types of binding interaction with targets.

Molecular Docking technique is useful component in the computational drug design. It is an automatic processor algorithm that defines how a molecule will bind in the active site of a target. It is essential tool in the process of drug discovery and development in order to identify the drug like candidates from set of compounds. Hence it is essential to know and understand the basic computational tools used in drug discovery and design.

The proposed Course title is dealing with “**Computational Tools in Drug Design**” which covers various tools and techniques in Drug Design. It is one of the essential courses for UG, PG, students and Ph. D scholars as this course imparts and orients students about drug design tools with more emphasis on hands on training.

Scope: This course is designed to deliver essential knowledge of computational tools in drug design with practical emphasis.

Course Objectives: The main objectives of proposed course are to

1. Understand the basics of Drug Design and Discovery.
2. Know the various softwares, servers and databases in drug design.
3. Perform Molecular Docking

Course Outcomes: Upon the completion of course, students shall able to

1. Explain the process of drug discovery and drug design.
2. Discuss about various softwares, servers and databases in drug design.
3. Describe the role of molecular docking in development of new lead molecules.
4. Handle drug design related softwares, serves and databases.
5. Identify the suitable drug-like candidates using molecule docking.

Course Modules

(24 Hours)

Module No.	Title of the Module	Duration (Hours)
I	Drug Discovery and Drug Design	6
II	Computer Aided Drug Design	6
III	Molecular Docking Approaches	6
IV	Hands on Training on Drug Design Tools	6
V	Overview to Advanced Excel	

Syllabus

Modules	Topics	Hours
Module-I	Drug Discovery and Drug Design <ul style="list-style-type: none"> • Drug Discovery and Development Process • Approaches of Drug Design • QSAR: Concept, Applications • Molecular Modeling • Virtual Screening techniques • Network Pharmacology: Overview 	6 Hours
Module Outcomes: Upon the completion of this module students will be able to: <ol style="list-style-type: none"> 1. Explain the basic concepts of Drug Discovery and Drug Design. 2. Discuss about virtual screening techniques and network pharmacology. 		
Module II	Computer Aided Drug Design <ul style="list-style-type: none"> • Softwares and Servers Used in CADD • Informatics and Databases In Drug Design • Chem Draw and Its Applications • Drug Likeness and ADMET Studies 	6 Hours
Module Outcomes: Upon completion of this module the students will be able to: <ol style="list-style-type: none"> 1. List out various tools of computer aided drug design. 2. Draw the chemical structure of molecules using Chem Draw. 		

3. Evaluate the Drug Likeness and ADMET properties of compounds.		
Module III	Molecular Docking Approaches <ul style="list-style-type: none"> • Introduction • Molecular Docking softwares • Target Identification • Ligand Preparation • Molecular Docking Process • Result Analysis and Prediction of Binding 	6 Hours
Module Outcomes: Upon completion of this module the students will be able to: <ol style="list-style-type: none"> 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 IV	Hands on Training on Drug Design Tools <ul style="list-style-type: none"> • Drawing chemical Structures • Drug Likeness Screening • ADMET Studies • Targets Identification • Ligand and Protein Preparations • Molecular Docking and Results 	6 Hours
Module Outcomes: Upon completion of this module students will be able to: <ol style="list-style-type: none"> 1. Handle basic tools of Drug Design. 2. Evaluate drug like molecules on the basis of their physicochemical, pharmacokinetic properties and binding interactions. 		
Module V	Overview to Advanced Excel Section One - Make a Start with Excel <ul style="list-style-type: none"> • What is a Spreadsheet? • Excel Rows and Columns • Enter Text and numbers in a cell • Data Formatting - Font formatting, Number formatting, colour of a cell; centre text and numbers; Table formatting, Conditional formatting, Hide/Unhide; Sort / filter, paste special, Find and select • Text Functions Using: Mid/Search/Left/Right Functions; Using Trim/Clean/Upper/Lower Functions; Using Substitute/Text Functions; Using Trim/Clean/Proper/Dollar Function • Currency symbols in excel • How to save your work in excel 	6 Hours

Section Two - Excel Formulae

- The SUM Function
- How to multiply in excel
- Subtract and Divide
- Combine the Arithmetic Operators
- Formula Auditing
- The Average Function
- The Date & Time Function

Section Three - Microsoft spreadsheet Features

- Advanced Filters - Extracting Records with Advanced Filter; Using Formulas in Criteria
- Advanced Sorting - Sorting by Top to Bottom/Left to Right; Creating/Deleting Custom List; Sort by using Custom List
- How to Merge cells
- Data Import from Web, Text (Text to columns)
- Removing Duplicates
- How to use Auto fill in excel
- How to Sort data in excel
- Searching with MATCH and INDEX
- How to Create an Excel Template
- Data Forms in Excel
- Drop Down Lists in Excel
- Add your own Error Messages
- Array Formulas Intermediate Excel
- Frequency Distribution Intermediate Excel
- Hyperlinks in Excel

Section Four - Microsoft Excel Pivot Tables & Charts

- Excel Pivot Tables (Creating, Formatting Simple PivotTables), Creating / Modifying a PivotChart
- Create an excel chart
- Formatting Charts: Move and Resize your chart; Charts Styles and Layouts; Adding Chart Titles and Series Titles Legends / Lables
- Formatting / Renaming / Deleting Data Series; Changing the Order of Data Series; Chart Layout Panel in Excel
- Printing Charts
- Adding Data to a Chart;
- Create Pie chart in Excel

- Format Pie chart segments
- Create a 2D line Chart in Excel (Combo Charts – Secondary Axis)
- Format your Axis titles
- Predict the future with a Trendline chart
- Sparkline charts
- Section Five - Conditional Logic
- 'IF' Function
- Conditional Formatting in excel
- Statistical Functions:
- CountIF, Count IFS, SUMIF, SUMIFS, Averagelf, Averagelfs, Nested IF, IFERROR Statement, AND, OR, NOT; LARGER / SMALLER Functions (Colour coding & data rearrangement)
- Absolute Cell References

Section Six - Advanced Excel – Data Processing & LOOKUP Functions

- Reference other Worksheets
- LOOKUP Function: VLOOKUP/HLOOKUP Function in Excel; Index and Match; Creating Smooth User Interface Using Lookup; Nested VLookup; Reverse Lookup using Choose Function
- Arrays Functions - Array Formulas, Use of the Array Formulas; Basic Examples of Arrays (Using ctrl+shift+enter); Array with if, len and mid functions formulas; Array with Lookup functions; Advanced Use of formulas with Array.

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

1. Create & Edit worksheets
2. Process data sets using Outline, autofilter & pivot tables
3. Process data sets employing Excel Formulae & produce statistical results
4. Extract and modify data with search and replace, use conditional formatting to highlight specific data
5. Creates and format PivotTables & Charts
6. Validate data using LOOKUP features

Assessment:**25% Formative assessment:**

- Theory Assignment: 15 marks
- Experimental Case Studies: 10 Marks

75% summative assessment:

- Continuous Mode: 10 Marks
- Theory Exam (Objectives, Long Essay and Short Essay): 25 Marks
- Practical Exercises and Viva Voce: 40 Marks

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 Park 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 Ikovas 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: Students of B. Pharm, M. Pharm, and Ph. D Scholars.

Duration: 24 Hours

Fees/Charges: The course is offered to the students without any fee

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
- Placement assistance

Career Prospects:

- Drug Discovery Research
- Computational Chemistry



Highlights of the Course

- Introduction to basics of Drug Design and Discovery.
- Orientation to various software, servers & databases employed in drug design.
- Insight into Molecular Docking approaches, Result Analysis & Prediction of Binding
- Hands-on training on Drug Design Tools