6-month Computational Drug Design Diploma Course (detailed Content) under Department of Pharmaceutical Chemistry

Summary

This diploma in computational drug design is designed to provide students with a comprehensive understanding of the principles and techniques used in modern drug discovery. Students will learn about molecular modeling, structure-based and ligand-based drug design, computational tools, and case studies of successful drug design projects. The research project component of the program provides students with hands-on experience and an opportunity to apply the skills and knowledge gained in the program. Upon completion of the program, students will be equipped with the skills and knowledge required to pursue a career in the field of computational drug design, including roles in academic research, pharmaceutical industry, and biotech startups.

Rules and regulations for attending the Computational Drug Design Diploma Course:

• **Eligibility:** Students must have a bachelor's degree in a relevant field or equivalent work experience in related discipline after bachelor's.

• **Admission:** Students must apply for admission and be accepted into the program.

• **Attendance:** Students must attend all lectures, labs, and workshops as per the course schedule.

• **Grading:** Students will be graded on their performance in assignments, quizzes, exams, and research projects.

• **Plagiarism:** Plagiarism in any form will not be tolerated and will result in disciplinary action.

• **Code of Conduct:** Students must adhere to the institution's code of conduct and behave in a professional manner.

• **Academic Integrity:** Students must always maintain academic integrity and avoid any unethical practices.

• **Fees:** Students must pay the required fees for the program as per the approved fee structure.

• **Withdrawal:** Students can withdraw from the program before the specified deadline, but no fee will be refunded.

• **Certificate/Diploma:** Students who complete the program successfully will be awarded a certificate/diploma.

Note: To attend this diploma course, students are required to have a personal laptop with the following minimum specifications:

Processor: Intel Core i5 or equivalent
RAM: 8 GB or higher
Hard Disk: 256 GB or higher
Graphics: Dedicated GPU with at least 2 GB of VRAM
Display: 14 inches or larger with at least 1920x1080 resolution
Operating System: Windows 10 /11

This is to ensure that students have a suitable computing environment for running the computational tools and software used in the course.

Short Content of Syllabus

- **First 3 Months:**

Course 1: Introduction to Drug Design and Molecular Modeling (2 credits)

• Principles of drug discovery process
• Pharmacokinetics and pharmacodynamics of drugs
• Importance of computer-aided drug design in modern drug discovery
• Introduction to molecular mechanics and quantum mechanics
• Molecular dynamics simulations
• Docking and scoring
• Analysis and visualization of molecular structures

Course 2: Structure-Based and Ligand-Based Drug Design (2 credits)

• Protein-ligand interactions
• X-ray crystallography and NMR spectroscopy
• Homology modeling
• Structure-based optimization
• Quantitative structure-activity relationship (QSAR)
• Pharmacophore modeling
• Molecular similarity analysis
• Virtual screening

Course 3: CADD Case Studies and Computational Tools (2 credits)

• Successful drug design projects in various therapeutic areas
• Rational drug design using structure- and ligand-based approaches.

• Drug repurposing and drug combination studies
• Introduction to cheminformatics tools and databases
• Data visualization and analysis
• Machine learning in drug discovery
• Introduction to artificial intelligence and deep learning in drug discovery

- **Next 3 Months:**

Course 4: Research Project (4 credits)

- Students will work on a research project under the guidance of a faculty member or mentor.
- The project can be in any area of computational drug design, such as molecular modeling, docking, QSAR, or machine learning.
- Students will be expected to submit a final report and give a presentation on their research findings.
- This project will be evaluated by an external examiner.

Note: The diploma course is shorter and more focused on specific topics related to computational drug design. The total credit hours for this course would be 10, with 6 credits devoted to coursework and 4 credits devoted to the research project.

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Detailed Content of Syllabus

- **First 3 Months:**

Course 1: Introduction to Drug Design and Molecular Modeling (2 credits)

Week 1: Principles of drug discovery process
• Overview of drug discovery and development
• Preclinical and clinical trials
• FDA approval process

Week 2: Pharmacokinetics and pharmacodynamics of drugs
• Drug absorption, distribution, metabolism, and excretion (ADME)
• Mechanisms of drug action
• Drug-target interactions

Week 3: Importance of computer-aided drug design in modern drug discovery
• Introduction to computer-aided drug design (CADD)
• Advantages of CADD in drug discovery
• Types of CADD tools and techniques

Week 4: Introduction to molecular mechanics and quantum mechanics
• Basics of molecular mechanics and force fields
• Introduction to quantum mechanics and density functional theory (DFT)
• Application of molecular mechanics and quantum mechanics in drug design

Week 5: Molecular dynamics simulations
• Overview of molecular dynamics (MD) simulations
• Techniques for MD simulations
• Analysis and visualization of MD simulation data

Week 6: Docking and scoring.
• Principles of molecular docking
• Docking algorithms and scoring functions
• Evaluation of docking results
• Analysis and visualization of docking results

Course 2: Structure-Based and Ligand-Based Drug Design (2 credits)

Week 1: Protein-ligand interactions
• Types of protein-ligand interactions
• Structure and function of proteins
• Ligand design and optimization

Week 2: X-ray crystallography and NMR spectroscopy
• Introduction to X-ray crystallography and NMR spectroscopy
• Principles of protein structure determination
• Applications of X-ray crystallography and NMR spectroscopy in drug design

Week 3: Homology modeling
• Basics of homology modeling
• Sequence alignment and homology detection
• Model refinement and evaluation

Week 4: Structure-based optimization
• Lead optimization strategies
• Structure-based design of novel compounds
• Structure-activity relationship (SAR) analysis

Week 5: Quantitative structure-activity relationship (QSAR)
• Principles of QSAR
• Molecular descriptors and their selection
• Statistical methods for QSAR

Week 6: Pharmacophore modeling and molecular similarity analysis
• Basics of pharmacophore modeling
• Generation and validation of pharmacophore models
• Molecular similarity analysis and its applications
• Virtual screening techniques

Course 3: CADD Case Studies and Computational Tools (2 credits)

Week 1: Successful drug design projects in various therapeutic areas
• Case studies of successful drug design projects
• Therapeutic areas and drug targets

Week 2: Rational drug design using structure- and ligand-based approaches.

• Integration of structure-based and ligand-based approaches in drug design
• Case studies of rational drug design

Week 3: Drug repurposing and drug combination studies
• Introduction to drug repurposing
• Strategies for drug combination studies
• Case studies of drug repurposing and combination studies

Week 4: Introduction to cheminformatics tools and databases
• Chemical databases and their applications in drug discovery
• Structure search and substructure search
• Data curation and management

Week 5: Data visualization and analysis
• Basics of data visualization
• Techniques for data analysis
• Applications of data visualization and analysis in drug discovery

Week 6: Machine learning in drug discovery and introduction to artificial intelligence and deep learning
• Basics of machine learning and its applications in drug discovery
• Introduction to artificial intelligence and deep learning
• Applications of AI and deep learning in drug discovery

- **Next 3 Months:**

Course 4: Research Project (4 credits)

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