B. PHARMACY
Syllabus  •  Semester-8

Elective subject-5 name with code: 13PH0807 Computer-Aided Drug Design

Course Objective
This subject is designed to provide detailed knowledge of the rational drug design process and various techniques used in the rational drug design process.

Course Outcomes
Upon completion of the course, the student shall be able to
1. Design and discovery of lead molecules.
2. The role of drug design in the drug discovery process.
3. The concept of QSAR and docking.
4. Various strategies to develop a new drug-like molecule.
5. The design of new drug molecules using molecular modelling software.

Teaching and assessment scheme

<table>
<thead>
<tr>
<th>Teaching Scheme (Hours)</th>
<th>Credits</th>
<th>Theory/ Tutorial Marks</th>
<th>Practical Marks</th>
<th>Total Marks</th>
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<tr>
<td>Theory</td>
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<td>Practical</td>
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Theory syllabus

Unit-1

Unit-2
Quantitative Structure-Activity Relationship (QSAR): SAR versus QSAR, History and development of QSAR, Types of physicochemical parameters, experimental and theoretical approaches for the determination of physicochemical parameters such as Partition coefficient, Hammett’s substituent constant and Tafts steric constant. Hansch analysis, Free Wilson analysis, 3D-QSAR approaches like COMFA and COMSIA.

Unit-3

Unit-4
Informatics & methods in drug design: Introduction to Bioinformatics, chemoinformatic. ADME databases, chemical, biochemical and pharmaceutical databases.

Unit-5

Tutorials will be based on the above syllabus.

Teaching hours: 15 Hours

Recommended references (Latest edition)

www.marwadiuniversity.ac.in