SACRED HEART COLLEGE Autonomous

DEPARTMENT OF CHEMISTRY
SACRED HEART COLLEGE (AUTONOMOUS)
THEVARA, KOCHI – 682013
Tel: 0484 2663380, Fax: 0484 2663813, www.shcollege.ac.in

Value Added Course

Course Code: 17CHEVAC01

Course Title: "Molecular Modelling and Molecular Docking"

Eligible Students: MSc Chemistry/Pharmaceutical Chemistry Semester-IV Students.

(30 Hours)

This course enables the students to have a better understanding and develop skill in Computational Chemistry and Drug Design

Learning objectives

The objective of the course is to provide a strong focus on the practical aspects of computational chemistry and computer-assisted drug design. The following are the objectives of the course:

- Ligand-based drug design approaches and examples.
- The impact of pharmacophore modelling in drug design.
- Structure-based molecular design approaches and examples.
- Methods and applications of quantitative structure activity relationships (QSAR).
- 3D database search strategies and their applications to molecular design.
- Modern structure-based and de novo molecular design approaches, including most recent developments, such as virtual high-throughput screening, docking and scoring.

Course Outline:

Unit I:

Molecular modeling: Introduction to molecular modeling, molecular methods.

Unit II:

Introduction to protein structure: Molecular visualisation softwares, Pymol/VMD.

Unit III:

Ligand-based drug design: Pharmacophore modeling in drug design.

Unit IV:

Computer-aided drug design (CADD): Introduction to computer-aided drug design (CADD) Introduction to molecular recognition and docking.

Unit V:

Quantitative Structure Activity Relationships (QSAR): Introduction to QSAR, Types of QSAR models, Applications.

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Reference

1. Asit K Chakraborti and Ramasamy Thilagavathi. Electronic Journal of Molecular Design, 2003, 2
2. Daniel Seeliger and Bert L.Groot. Journal of Computer Aided Molecular Design. 24, 417422, 2010.
3. Computational Medicinal Chemistry for Drug Discovery, P Bultinck P DeVinter
4. Computer Aided Drug Design, Pope&Perruns, Academic Press NY
5. Computer Aided Drug Design, TJ PERUN7 CL Propst, Marcel& Dekker, 2007

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