- Quizzes
- End semester university examination.

Keywords:

Chemical Technology; Society; Energy; Polymer; Pollutants.

Course Code: CHEMISTRY –SEC-4
Course Title: Chemoinformatics
Total Credits: 04 (Credits: Theory-02, Practicals-02)
(Total Lectures: Theory- 30, Practicals-60)

Objectives:

The aim of the course is to introduce the students to computational drug design through structure-activity relationship, QSAR and combinatorial chemistry. The students will learn about the target analysis, virtual screening for lead discovery, structure based and ligand based design method and the use of computational techniques, library preparation and data handling.

Learning Outcomes:

By the end of the course, the students will be able to:

- Have a comprehensive understanding of drug discovery process and techniques including structure-activity relationship, quantitative structure activity relationship and the use of chemoinformatics in this, including molecular modelling and docking studies.
- Appreciate role of modern computation techniques in the drug discovery process and perform their own modelling studies.

Unit 1:

Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular modelling and structure elucidation.

(Lectures: 2)

Unit 2:

Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

(Lectures: 2)

Unit 3:

Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

(Lectures: 6)

Unit 4:

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity.

(Lectures: 6)

Unit 5:

Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design

(Lectures: 6)

Unit 6:

Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Chemoinformatics in Drug Design.

(Lectures: 8)

Practical:

(Credits: 2, Laboratory periods: 60)

1. Overview of Rational Drug Design, Ligands and Targets

2. In silico representation of chemical information

i. CIF IUCr Crystallographic Information Framework
ii. CML Chemical Markup Language
iii. SMILES -- Simplified Molecular Input Line Entry Specification
iv. InChi -- IUPAC International Chemical Identifier
v. Other representations

3. Chemical Databases and Data Mining

i. Cambridge Structural Database CCDC CSD
ii. Crystallographic Open Database COD
iii. Protein Data Bank PDB Ligand Explorer
iv. Chemspider
v. Other Data Bases

4. Molecular Drawing and Interactive Visualization

i. ChemDraw
ii. MarvinSketch
iii. ORTEP
iv. Chimera, RasMol, PyMol

5. Computer-Aided Drug Design Tools

i. Molecular Modeling Tools
ii. Structural Homology Modeling Tools
iii. Docking Tools and Screening Tools
iv. Other tools

6. Building a Ligand

i. Building ab initio
ii. Building from similar ligands
iii. Building with a known macromolecular target
iv. Building without a known macromolecular target
v. Computational assessment of activity and toxicity and drugability.

References:

1. Leach, A. R.; Gillet, V. J. (2007), **An introduction to Chemoinformatics**, Springer.
2. Gasteiger, J.; Engel, T. (2003), **Chemoinformatics: A text-book**. Wiley-VCH.
3. Gupta, S. P. (2011),**QSAR & Molecular Modeling**. Anamaya Pub.
4. Gasteiger, J. **Handbook of cheminformatics: from data to knowledge in 4 volumes,** Wiley.

Additional Resources:

1. Jürgen,B.(2004),**Chemoinformatics Concepts, Methods, and Tools for Drug Discovery**, Springer

Teaching Learning Process:

The course aims to introduce students to different cheminformatics methods and its use in drug research through practicals. It is a rather new discipline of science. It concerns with the applications of computer to solving the chemistry problems related to drug designing and drug discovery.

The course will give emphasis on active learning in students through a combination of lectures, tutorials and practical sessions. The underlying principles will be explained in lectures and the practicals will establish the understanding of these principles through applications to drug research.

Assessment Methods:

- Formative assessment supporting student learning in Cheminformatics practicals
- Summative assessment
- Review of a case study
- Exercise based on SAR and QSAR-Report
- Practical exam of five hours