Subject Code : P8BIE3A

CHEMOINFORMATICS

UNIT I

Computational chemistry-history-objectives-Computational techniques-software-databases-hardware and network-organization-Computers and chemical structures-chemical nomenclature-use and limitation of models and modeling- Computer graphics for structural analysis of small molecules.

UNIT II

Representation and manipulation of 2D and 3D structures-substructure-3D pharmacophore searching-Molecular descriptors-2D and 3D descriptors-data verification and manipulation-Computational models-deriving QSAR equations-designing a QSAR experiment-Statistical techniques-similarity methods-2D finger prints-similarity co-efficients-2D and 3D descriptors methods.

UNIT III

Selecting diverse set of compounds-cluster analysis-dissimilarity based selection methods-cell based methods-evaluation methods-Analysis of high-throughput screening data-data visualization-data mining methods-Virtual screening-drug likeliness-structural based virtual screening-prediction of ADMET properties-Combinatorial chemistry and ligand design-library enumeration-library design strategies-Lead structure discovery and development.

UNIT IV

Applications of quantum and molecular methods-Molecular mechanics for modeling of drugs-Quantum mechanics for modeling of drug structure-Molecular dynamic simulation in drug development process-QSAR to molecular graphics-Biocatalyst design and application.

UNIT V

Sources of chemical information-online resources-activity searching-synthesis modeling-trends and developments-Chemical genomics-advantages and limitation-chemical genetics-diversity based approach-In silico chemical genomics-Process optimization-Resources for chemical genomics (Pharmabase and MSDchem).

Reference Books

1. Chemometrics and chemoinformatics. Washington, DC: American Chemical Society, 2005.
2. Bunin, Barry A. Chemoinformatics: Theory, Practice, and Products. Dordrecht: Springer, 2007.
3. Bajorath, Juergen, ed. Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery. Totowa, N.J.: Humana Press, 2004.
4. Gasteiger, Johann; Engle, Thomas, eds. Chemoinformatics: A Textbook. Weinheim, Germany: Wiley-VCH, 2003.

5. Gasteiger, Johann, ed. Handbook of Chemoinformatics: From Data to Knowledge. Volume 4. Weinheim, Germany: Wiley-VCH, 2003.
6. Leach, Andrew R.; Gillet, Valerie J. An Introduction to Chemoinformatics. Dordrecht: Kluwer, 2003.
7. Oprea, Tudor I. Chemoinformatics in Drug Discovery. Weinheim: Wiley-VCH, 2005.
8. Pirrung, Michael C. Molecular Diversity and Combinatorial Chemistry: Principles and Applications. Amsterdam: Elsevier, 2004.
9. Ekins, Sean, ed. Computer Applications in Pharmaceutical Research and Development. Hoboken, N.J.: Wiley, 2006.
10. Ferenc Darvas, András Guttman, György Dormán. Chemical Genomics. Marcel Dekker Inc, New York, 2005.
11. John B. Taylor, Comprehensive Medicinal Chemistry (Volume I-VI). Pergamum Press, England, 2005.