20CY111 COMPUTERS IN CHEMISTRY

Hours Per Week :

L	T	P	C
3	-	-	3

Course Description and Objectives:

This course introduces the basics concept and role of computer in chemistry. Topics covered are Fundamentals of Computer, various operating system, number of tools to sketch the chemical structures, number of chemical database, basics of computational chemistry and basics to write the coding.

Course Outcomes:

Upon completion of the course, the student will be able to gain the knowledge and achieve the outcomes on :

COs	Course Outcomes
1.	Understand the basic functions of computer
2.	Analyze the various chemical databases
3.	Utilize the computational tools to solve the chemical problems
4.	Apply various computational methods to solve chemical problems
5.	Analyze the concept of python script for chemical calculations

Unit - I :

Introduction to computer: Introduction and Fundamentals of Computer, MS office and applications, basic commands in Linux, handling Cookies.

Unit - II :

Chemistry softwares: Introduction to Chemdraw, Chemsketch tools to draw chemical structures, Convert chemical name to structure and vice versa, Chemical data bases like CAS, Pubmed, Chemspider, ZINC, PDB, Drug Bank, Super Drug and its usage, various file format of chemical structures (SMILES, PDB, Mol, SDF and .com), Elementary structural features such as bond lengths, bond angles, dihedral angles etc., of molecules.

Unit - III:

Density functional theory (DFT): Introduction and scope of computational chemistry, ab initio methods, Basics of Density functional theory (DFT), Creating chemical Structures and visualization software like Gauss view, Pymol. Introduction to docking and scoring.

Unit - IV:

Molecular mechanics: Introduction to molecular mechanics; force fields; comparison of popular force fields, Introduction to Molecular dynamics, The Born-Oppenheimer approximation, potential energy surfaces, local and global minima, transition states and theory. (7 hours)

Unit - V :

Python : Introduction, Computer applications in Chemistry: Development of small computer codes using python involving simple formulae in chemistry such as calculate molecular weight, van der Waals equation, and kinetics.

Text Books:

1. Computational Chemistry by A. C. Norris, John Wiley

2. INTRODUCTION OF PYTHON by Prof. Vishwajit K. Barbudhe

3. The ABC of DFT by Kieron Burke.

4. Atkins' Physical Chemistry: International Eleventh Edition.

5. Elements of physical chemistry by B.R. Puri and L.R. Sharma, 2013 ed.