Course Code	Course Name	Credits
26CH951	MOLECULAR MODELING AND DRUG DESIGN	02

Course Description

This course provides practical and computational training in molecular modeling, structural chemistry, and computer-aided drug design. It covers the study of bond lengths, molecular orbitals, conformational analysis, electron density, electrostatic potential maps, dipole moments, molecular stability, and resonance energy calculations of organic and inorganic molecules.

Course Objectives

- To introduce students to molecular modeling and computational chemistry tools for studying molecular structure, geometry optimization, and electronic properties.
- To develop understanding of chemical bonding concepts through the analysis of bond lengths, molecular orbitals, electron density, and electrostatic potential maps.
- To provide practical training in conformational analysis, molecular stability, dipole moments, and resonance energy calculations of organic and inorganic molecules.

Skill Enhancement Outcomes

Upon successful completion of this course, the learner will be able to:

- Develop computational skills in molecular visualization, structure optimization, and conformational analysis using modeling software.
- Enhance the ability to interpret electronic properties such as molecular orbitals, charge distribution, dipole moments, and resonance effects.
- Strengthen analytical skills in comparing molecular stability, acidity, and basicity across different chemical systems.
- Acquire practical expertise in ligand-based drug design and protein–ligand docking studies for pharmaceutical applications.

Course Content and Practical Training

- Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene.
- Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
- Perform a conformational analysis of butane.
- Visualize the electron density and electrostatic potential maps for LiH, HF, N2, NO and CO and comment. Relate to the dipole moments.
- Relate the charge on the hydrogen atom in hydrogen halides with their acid character.
- Compare the gas and aqueous phase basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule.
- Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide
- Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- Arrange 1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2- pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- Ligand-based drug designing: Protein-ligand docking.
- Molecular modelling of drug-receptor interaction: Prediction of active site in receptor, building small molecules, ADME Predictions.

Learning outcome

Upon successful completion of this course, students will be able to apply molecular modeling and computational chemistry techniques to analyze molecular structure, bonding, stability, electronic properties, and drug–receptor interactions for chemical and pharmaceutical applications.