Course Type	Course Code	Name of Course	L	T	P	Credit
DP	NCYC523	Computational Chemistry Lab	0	0	3	1.5

Course Objective

- The idea of practical classes is to provide students an exposure to methods, softwares, and practices associated with the computational chemistry and its application in various fields.
- The students will learn basics of computational chemistry and its various applications in a variety of fields.

Learning Outcomes

- The students will have a hands-on experience with problems of different computational complexity and use the standard methods and softwares to solve them.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Basis set dependence of energy of Quinoline and Isoquinoline in DFT Calculations	03	DFT based optimization type calculation and its basis set dependence
2	Charge Distribution in Quinoline and Isoquinoline	03	Impact of Functional Group Substitutions on the Charge Distribution in Quinoline and Isoquinoline
3	Nucleophilic Substitution of Hydroxide Ion in Chloromethane	03	Mechanistic Insights into SN2 Reactions; transition state search
4	Identify unknown molecule using computed IR and NMR spectra	03	Estimation of the IR and NMR spectra of several small organic molecules and use the calculated spectra to help identify an unknown molecule.
5	Estimate the amount of ring strain in cycloalkanes	03	Effect of ring strain on the energy of the molecule
6	Compute and visualize molecular orbitals of several molecules	03	MO-LCAO picture of bonding and symmetry of electronic wave functions.
7	Docking of ligands in binding pocket	03	Rigid and Flexible docking Techniques, Structure-Based Virtual Screening (VS)
8	Diffusion coefficient of water using Molecular Dynamics Simulations	03	Different water models used in Molecular Dynamics
9	Molecular Dynamics Simulation of a small protein in water	03	Conformational behavior of protein in water
10	Molecular Dynamics Simulation of a small protein with ligand	03	Ligand binding affinity calculations using MM-GBSA
11	quantitative structure-activity relationships (QSAR)	03	relationship between chemical properties and biological activities.
12	Numerical solutions of ordinary differential equations	03	Usage of matlab / python for solving ordinary differential equations numerically with different boundary conditions
13	Numerical solutions using Newton-Raphson method	03	python/C++ code for finding real roots of a nonlinear function using Newton-Raphson method.

14	Ploting of both analytical functions and raw data	03	Usage of matplotlib / matlab for plotting purposes
Total		**42L**	

Text Books:

1. The Art of Molecular Dynamics Simulation, by D. C. Rapaport , Cambridge University Press; 2nd edition (1 April 2004),ISBN-10 : 0521825687.
2. Computational Chemistry Using the PC. Donald W. Rogers ,Wiley-Interscience; 3rd edition

Reference Books:

1. Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, By David Young, Wiley-Interscience; 1st edition, ISBN-10 : 0471333689