Course Type	Course Code	Name of Course	L	T	P	Credit
DE	NCYD542	Numerical Analysis and Methods in Chemistry	3	0	0	3

Course Objective
The course is aimed to introduce the basics of theoretical and numerical methods for computer simulation of model systems. It also intends to develop elementary programming skills in C++ to enable them write short programs for performing scientific calculations.
Learning Outcomes
• At the end of the course, the learners should be able to: • Write short, simple programs in C++ • The students should be able to perform basic molecular modeling for various chemical and physical problems using standard software's such as TeraChem, Gaussian, NAMD, AMBER, etc. The student should be also understand simulated results and correlate with corresponding experimental observations.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Errors in Chemical Analyses, Random Errors in Chemical Analysis, Statistical Data Treatment and Evaluation, Sampling. Standardization, and Calibration. Usage of packages (e.g. ORIGIN; EXCEL) for data analysis. Curve Fitting: Linear and Non-linear fitting of data.	9L	This module will emphasize on the type of errors in measurements, their treatment and reporting of data by obtaining best fits to the dataset through curve fitting.
2	Introduction to programming languages (C++): data types, arrays, functions, classes and objects, constructors and destructors, function overloading, operator overloading; Basic numerical analysis: solution of linear and nonlinear equations.	15L	Brief introduction to write C++ programs which is implemented in cheminformatics, bioinformatics, computational chemistry and computational biology.
3	Review of Basic Concepts: Length and Time Scales, Intermolecular Interactions and Potential Energy Surfaces, Classical Molecular Dynamics (MD): Langevin and Newtonian equations of motions, Various integration algorithms, and Force calculations. All atom and ab-initio molecular dynamics, Quantum mechanics/molecular mechanics (QM/MM) approaches. Use of various commercially available molecular modelling and simulation software (NAMD, AMBER, TeraChem, and GAUSSIAN).	18 L	Comprehensive understanding of specific interactions among different molecules that define the potential energy surface, in-depth understanding of the basic concepts involved in classical molecular dynamics which are crucial to design the simulations.
Total		**42**	

Text Books:

1) Elementary Numerical Analysis-An Algorithm Approach, S.D. Conte and C. De Boor, McGraw Hill, 1980.

2) Programming: Principles and Practice Using C++, Bjarne Stroustroup, Addison-Wesley Publisher, 2017.

Reference Books:

1) Understanding Molecular Simulation: From Algorithms to Applications, Berend Smit and Daan Frenkel, Academic Press, 2002.
2) Introduction to Computational Chemistry, F. Jensen, John, Wiley & Sons, 2nd Edition (2007).