Certificate programme -2022-23

Department of Chemistry

Morigaon College

Hands on Training of basic chemistry software

Course Duration – 30 Hours

Course credit- 3

Course Objectives

The Department of Chemistry, Morigaon College , offers a 30-hour certificate programme in Hands on Training on Basic Chemistry Software. This goal of this course are to teach students and researchers with chemistry as a major how to use a variety of open source chemistry tools. By the end of the course, participants will be able to efficiently use these software programmes to create chemical structures, generate names for them, and retrieve data on calculations of physical properties, calculations of three-dimensional molecular structures, spectroscopic signatures, predictions of chemical reaction pathways, molecular functional groups, and predictions of docking sites.

Learning outcomes

*Candidate will be able to generate and process simple and complicated chemical structures using ACD ChemSketch after successfully completing this module.

* The candidate will be able to analyse three-dimensional properties of molecules after successfully completing this module, which is extremely helpful in predicting their chemical and physical properties and can be used in advanced research work.

* Candidates who successfully complete this session will be able to use internet research tools effectively and search for relevant research papers more quickly.

*Candidates who successfully complete this module will be able to use docking to study drug-receptor interactions. The understanding of these interactions is a crucial prerequisite for the contemporary drug discovery process.

Eligibility

All B.Sc. final-year students who are honours in chemistry are eligible.

Evaluation Process·

Following the completion of each module, students will be evaluated through theoretical assignments, projects, and practical exams. Certificates will be given to all successful candidates.

Key characteristics of the certificate programme include:

- Theory and practical sessions that follow the curriculum
- Lectures that cover the whole download and installation process for these softwares.
- Training in real-world use of all these programmes
- Candidates will be able to utilise these open source programmes on their own after completing the course.
- The successful candidates will receive a certificate.

Module 1 (4 hours)

ACD ChemSketch software:– A description, the downloading and installation process. Drawing different chemical structures (acyclic, cyclic, polycyclic, and heterocyclic), generating names from structures, translating a molecule's name into its structure, and computing physical properties like density, molecular weight, refractive index, bond angles, bond lengths, and dihedral angles from a structure's structural formula.

Module 2 (5 hours)

Cambridge ChemDraw Ultra software– A description, the downloading and installation process, Drawing different chemical structures (acyclic, cyclic, polycyclic, and heterocyclic), creation of nomenclature, translation of names into molecular structures, and derivation of physical attributes from structural formulae such density, molecular weight, and refractive index. Prediction of 1H, 13C NMR from molecular structure, Using templates, bioarts, and drawing the structure of larger molecules like proteins, carbohydrates, and RNA/DNA Software comparison between Cambridge ChemDraw Ultra and ACD ChemSketch.

Module 3 (8 hours)

Chem3D software:- A description, the downloading and installation process, molecular 3D structure, numerous models of 3D structure, and transformation of 2D structure into 3D structure, extension of files, metric coordinates, diffraction angles, Molecular electrostatic potential (MEP) surface, electrostatic potential (ESP) surface, and solvent accessible surface calculations are all related to energy minimization. computations of atomic charge, MM2 calculations, Huckel calculations, and the computation of dipole moments MM2 computations are used to calculate the UV and IR spectra.

Module 4 (5 hours)

Search of a chemical database online introduction utilizing keywords to identify and download research papers using Sci-reaction, finder's product, reactant, and Scopus, Science Direct, and Google Scholar databases. a description of End Note and its uses.

Module 5 (8 hours)

Chimera 1.12 software:- A description of the Chimera software preparing ligands and proteins for docking, searching protein data banks for structures, and protein-ligand docking websites that do ligand binding analyses simple molecules are docked over the active site of proteins, and the outcomes of the docking are analysed.

Approved