

## **ADD ON COURSE**

### **DEPARTMENT OF CHEMISTRY**

### **NALBARI COLLEGE**

**Name of the Course: Learning Some Basic Chemistry Softwares**

**Duration :** 32 hours

**Course Code :** CHE-Ad-on-01

#### **Course Committee**

**Chief Patron:**

Dr. Kamal Nayan Patowary  
Principal, Nalbari College  
Nalbari

**Chairperson:**

Dr. Dhiraj Talukdar  
HoD, Dept. of Chemistry  
& IQAC Coordinator

**Coordinator:**

Dr. Purabi Sarmah

**Course Designed by:**

Dr. Purabi Sarmah

**Asst. Coordinator:**

Dr. Pranita Bora

#### **Faculty instructors**

1. Dr. Dhiraj Talukdar (DT)

2. Dr. Rupam Sarma (RS)

3. Dr. Purabi Sarmah (PS)

4. Dr. Pranita Bora (PB)

5. Dr. Ranjan Jyoti Sarmah (RJS)

Librarian, Nalbari College

## Some Basic Chemistry Softwares

DURATION: 32 hours

CHE-Ad-on-01

New educational policy (NEP) 2020 demands that our undergraduate students should be given a better opportunity in learning some additional skill-based knowledge apart from the traditional subjective knowledge that are already in the curriculum. This add on course is designed to help our B.Sc. students to learn various open-source chemistry softwares which are very much essential for sustainable carrier in Chemistry in future.

### Objective:

This course is aimed at providing hands on training of drawing simple or complex chemical structures, reaction schemes, graphical representation of data, molecular modelling and various other analytical tools which are indispensable for a chemistry student or a researcher.

### COURSE DETAILS:

#### Module I: Learning Cambridge Chem Draw Ultra software (8 hours)

This chemical software is a molecular editor which is scientifically designed for drawing chemical as well as complex biological structures. It helps to create electronic description of molecules, graphics, reaction schemes etc. necessary for producing publication standard quality. This software permits us to draw structural representation of various organic molecules such as aromatics, bicyclic systems, polyhedra, phenyl rings, cycloalkanes, stereochemical, conformational and supramolecular structures etc. Orbital structures can also be drawn with the help of this software. It also enables one to draw various biological structures such as DNA, RNA, sugars, amino acids and various necessary bio arts with the help of the templates incorporated in the software.

This module include:

- Introduction
- Download and installation
- Proper Guidance and hands on training of drawing a variety of chemical structures

- Drawing of 3D molecular structures.
- Chemical structure to name conversion and vice-versa.
- NMR spectrum simulation (Both  $^1\text{H}$  and  $^{13}\text{C}$  NMR)
- Mass spectrum simulation
- Practice task to students

### Module II: Learning ACD Chem Sketch freeware (7 hours)

This ACD/Chem Sketch Freeware is a comprehensive chemical drawing tool that allows us to draw a wide range of chemical structures including organometallic compounds, polymers and Markush structures as well. This software also allows us to calculate various molecular properties of the target molecule. 2D and 3D view of the drawn molecule can also be accessed through this software.

This module include:

- Introduction
- Download and installation
- Hands on training of drawing a variety of chemical structures
- Accessing 2D and 3D view of the target molecule and their comparison
- Calculation of molecular properties such as molecular weight, density, molar refractivity etc.
- Practice task to students

### Module III: Learning Origin Lab software (8 hours)

Origin Lab is the most preferred data analysis and graphing software used by the students, researchers, scientists and academia worldwide. This user-friendly software provides advance customized features which can be applied in displaying various analytical results. This interface facilitates data analysis, statistical analysis, exploratory analysis, peak analysis etc. A wide category of publication quality graphs can be produced using this software.

This module includes

- Introduction
- Download and installation process
- Drawing various graphs from the raw data
- high quality graphs export
- batch plotting

- 3D graph plotting
- statistical graph plotting, descriptive statistics
- Curve fitting and peak fitting, peak analysis, peak identification and integration.
- baseline correction.

#### **Module IV: Introduction to e-resources and their utilization (7 Hours)**

This course module allows the participants to acquire knowledge of accessing various e-resources those can be availed through various platforms such as Google Scholar, Swayam (Study Webs of Active Learning for Young Aspiring Minds), NPTEL (National Programme on Technology Enhanced Learning), N-list (National Library and Information services) programme, e -PG Pathshala etc. Study materials and many other relevant information in the field of Chemistry can be gathered through these platforms which will make them updated, competent and focused in their future course of action.

Important features of this module are:

- Searching and downloading of research paper through various platforms using keywords
- Online structural database search, product search through CSD (Cambridge Structural database) and CCDC (Cambridge Crystallographic Data Centre) search
- Writing of dissertation reports
- Use of End note and foot note for putting references etc.

**No of seats: 30**

**Course fee: Free**

**Resources:** Necessary computer facilities and softwares would be made available to students for smooth conduction of the add on course. Hands on training will be imparted by the competent faculty members of the Chemistry Department of Nalbari college as well as by experienced experts from other educational institutions.

#### **Learning outcome of the course:**

By completing this course, a student would be able to acquire basic knowledge of drawing simple and complex chemical structures, able to depict schemes, flow charts, reaction pathways, graphical representations, etc. They also would

be able to present and analyze various analytical data and practical findings in the form of project/dissertation reports or can be reported in the form of power point presentation.

**Evaluation and Certification: (2 hours)**

Students' performance and learning outcome of the course will be assessed by giving them practical assignments, group activities, projects, seminars etc. After completion of course all successful candidates will be awarded with certificates.