Diamond Jubilee Celebration
1961–2021

1961 - 2021

THE CHEMICAL SOCIETY
DEPARTMENT OF CHEMISTRY
SRI VENKATESWARA COLLEGE
UNIVERSITY OF DELHI
PRESENTS

SKILL-ENHANCEMENT WORKSHOP

ON

"DRAWING, ANALYSIS & COMPUTATIONAL SKILLS: SCIENTIFIC-SOFTWARES FOR EDUCATION, RESEARCH & PUBLICATION"

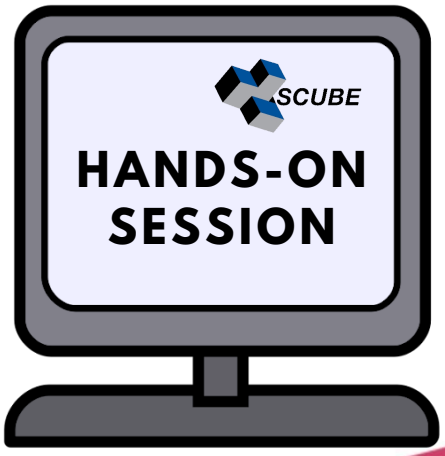
ChemDraw Professional, Chem 3D, Signals Notebook, MNOVA, Gaussian 16, Gauss view 6

On 7 October 2021 & 8 October 2021
(2 pm-6 pm)

Open for Science Undergraduates, Post-graduates and Research scholars

E-certificates shall be issued to all participants.

Last date of registration (Free registration): 5 October 2021



In collaboration with
Scube Scientific Software Solutions

SCUBE

Platform: Teams

LEARN FROM THE EXPERTS

REGISTER NOW!

CLICK HERE

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OBJECTIVES

This hands-on, interactive skill enhancement workshop is aimed at imparting skills on the use of various scientific softwares that are essential for students or researchers with chemistry as a major subject.

This skill enhancement workshop will focus on inquiry-based learning enhanced by computational thinking with content and practice to assist students to incorporate modeling at all levels of learning.

At the end of the workshop, participants will be able to use these softwares for drawing chemical structures, generation of their names, retrieve information about physical properties calculations, three-dimensional molecular structure calculations, spectroscopic analysis, chemical reaction pathways prediction, molecular functional groups, docking sites predictions, and other parameters efficiently.

The hands-on activities will expose participants to the basics of computational thinking, modeling, and data analysis.
We desire to have participants from a broad range of disciplines, including, but not limited to, chemistry, physics, computer science, mathematics, and the physical and life sciences.

Designing and drawing of chemical structures
ChemDraw Professional, Chem 3D & Signals Notebook

Analysis of combined NMR, LC/GC/MS and Electronic & Vibrational Spectroscopy data
MNOVA

Computation, predict energies & electronic structure modeling
Gaussian 16 & Gauss View 06

SALIENT FEATURES OF SKILL ENHANCEMENT WORKSHOP

- Theory and practical session
- Demonstration including the entire process of downloading and installation of these softwares.
- Hands-on training on all these softwares.
- At the end of the workshop, candidates will be able to use these softwares independently for their work.
- E-certificates shall be issued to all participants.
- No registration fee.

Softwares used

SCUBE SCIENTIFIC SOFTWARE SOLUTIONS

This workshop is conducted in collaboration with Scube Scientific Software Solutions, which is a renowned company engaged in distribution of scientific softwares used in fields like Computational Chemistry, Mathematical Modeling, Statistical Analysis, Data Mining amongst many others. Established in 2004, they have collaborated with global companies like Gaussian Inc., Wolfram Research Inc. to deliver tailor-made software solutions across India and other SAARC countries – in a bid to make world-class scientific software available to Indian researchers for their benefit.

01

CHEMDRAW

Created by PerkinElmer Informatics, ChemDraw is a Chemical Drawing program that allows users to draw molecular structures and other diagrams associated with Chemistry. Often considered the gold standard in chemical drawing, its powerful features enable users to create beautiful images ranging from simple molecules to complex macromolecules in a matter of minutes.

02

CHEM 3D

Chem3D is also a chemical drawing software and as the name suggests, it can be used to render colourful 3D structures. It can also be used to convert a 2D structure created with ChemDraw into its 3D – hence, it supplements ChemDraw. The structures thus produced can be used in presentations, posters, websites etc.

03 SIGNALS NOTEBOOK

A 'future-proof' electronic notebook solution, Signals Notebook is a software that can be used for almost all branches of science. With a simple and modern user interface, it is easy to learn and easier to use. By enhancing collaboration, improving workflow and lab automation, it leads to increased productivity and data transparency.

04 MNOVA

Almost an essential in Analytical Chemistry, this software developed by Menstrelab Research aids in the processing and analysis of combined NMR, LC/GC/MS and Electronic & Vibrational Spectroscopy data. Using three plugins Mnova NMR, Mnova ElViS and Mnova MS, the software covers a plethora of techniques like mixtures analysis, reaction monitoring, quantitation, chemical shift prediction, screening, verification as well as physico-chemical properties prediction apart from spectroscopy.

05 GAUSSIAN 16

A general purpose computational chemistry software, Gaussian 16 is an update of a long series of Gaussian softwares that offers state-of-the-art facility for electronic structure modelling. The ability to make reliable model with modest system requirements sets this software apart. The provision of a wide variety of methods makes it suitable for a broad range of chemical conditions, problem sizes and compounds.

06 GAUSSVIEW 6

GaussView 6 is the latest iteration of a graphical interface used with Gaussian. It aids in the creation of Gaussian input files, enables the user to run Gaussian calculations from a graphical interface without the need of using a command line instruction, and helps in the interpretation of Gaussian output (e.g., you can use it to plot properties, animate vibrations, visualize computed spectra, etc.)

SCHEDULE

DAY 1: THURSDAY, 7 OCTOBER 2021

ChemDraw Professional

- **Preference and Settings** - Customizing toolbars and HotKeys, Working with colors and Document Settings.
- **Page Layout** – The Drawing Area, Document Types, Saving page setups, Tables.
- **Shortcuts and HotKeys** – Atom, Bond and Modifying hotkeys, Shortcuts, Nicknames, Defining R group, 3D cleanup.
- **Basic Drawings in ChemDraw** - Changing Bond Orders, Adding atom labels, Drawing Rings, Fisher Projections, Perspective Drawing, Newman Projections, Stereochemistry.
- **Structure=Name** – Structure> Name, Name> Structure, Adding structures to dictionary.
- **Advanced Drawings in ChemDraw** – Organometallic drawing, Reaction. Mechanism drawing, advanced features.
- **Templates** – Creating your own templates, modifying the templates.
- **Drawing Monomer Sequences** – Amino acid sequences, DNA/RNA Sequences, HELM Notations, Copying/Pasting Sequences, expanding sequences, Contracting labels, Pasting sequencing, Disulfide Bridge, Lactam Bridges, Chem Bio Arts.
- **Advanced Drawing Tools** – Coloring objects, Labels, Attachment Points, Atom numbering, Mass Fragmentation, Drawing Reactions, Stoichiometry, Defining Nicknames, ChemNMR, TLC/Gel electrophoresis Drawings, Structural Analysis, Chemical properties

Chem3D

Building a model and rotations, Generating bond length/angles/dihedral angles, Trans to Cis isomers, Steric energy of eclipsed and staggered conformers, Overlaying model to compare structural similarities, HOMO-LUMO visualization, visualizing partial charges/lone pair electrons/van der Waals radius, Conformational Analysis, Molecular Dynamics, Stereochemistry, saving a movie file.

Signals NoteBook

Making notebook and experiments; creating group and sharing the experiments, chemical details, ChemDraw embedded notebook, working with MS Office in ELN and exporting.

Q&A session

Mnova

- **Mnova NMR**: Basic processing of raw data (baseline correction, Phase correction, zero filling etc), Peak picking, integration, Automatic multiplet analysis, Reporting. Introduction of Mnova MS, ElViS, qNMR, Predict, Assignment, Structure Elucidation.
- **Mnova MS**: Total ion Chromatogram, integration of peaks, UV-PDA/DAD traces, Elemental composition, molecular match.
- **Mnova ElViS/Predict/Assignment:** Processing of NIR/UV-Vis data, Structure drawing and predicting the 1d and 2d spectra, Assigning a peak to structure.
- **Structure Elucidation**

Q&A Session

SCHEDULE

DAY 2: FRIDAY, 8 OCTOBER 2021

Gaussian 16 & GaussView 6

1. **Introduction of Gaussian 16**
   What is Gaussian 16? Background of Electronic Structure Theory, Independent Particle Models, Model Chemistry, Basis Sets
2. **Drawing with GaussView 6**
   Point Group, Symmetry, Dock Atom, selection tools, working with proteins
3. **Input File & Output file**
   Setting up an input File in Gaussian 16 and GaussView 6, Reading the output file for Energy, optimization, Frequency and Transition State. Geometry Optimization
4. **Geometry Optimization:**
   Minimization, Geometry Optimization - Transition structure optimization, Reaction Path Following
5. **Frequency Calculations**
   Raman & IR frequency calculations
6. **Q&A Session**

LEARNING OUTCOMES

After successful completion of this module, candidates will be able to do generation and processing of simple and complex chemical structures.

The participants will be able to use ChemDraw Ultra for generation, processing and calculation of physical/chemical properties of simple and complex molecules.

The candidates will be able to study three-dimensional properties of molecules which are highly useful in prediction of their chemical/ physical properties and can be applied in advanced research work.

The candidates will be able to use online research tools efficiently and will be able to search research papers related to their topics more efficiently.

Candidates will be able to study drug-receptor interactions through docking. The knowledge of these interactions is a fundamental requirement for modern drug discovery process.

REGISTRATION

Enrollment in the workshop is limited and we require registration

Registration link: https://forms.gle/ujWLg56WosqL44k47

No registration fee is required

Note that from the organizers, you will also receive the download and installation instructions for softwares. Make sure you have it installed and briefly tested!