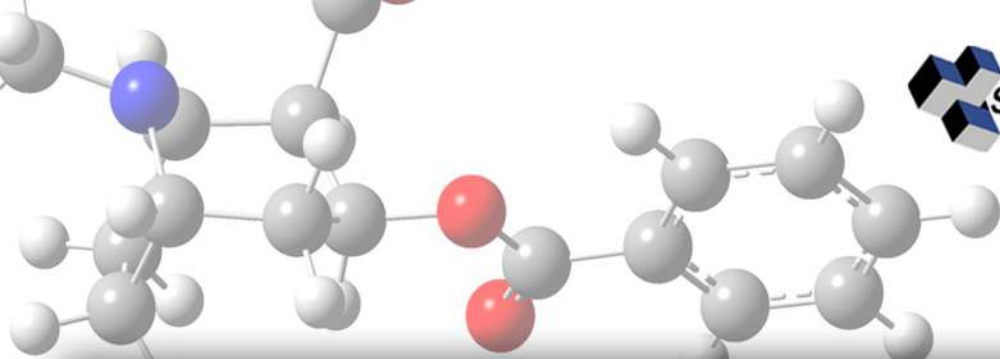


**SCUBE**TMSCIENTIFIC SOFTWARE SOLUTIONS PVT. LTD.
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Cloud-based Virtual Workshop:
Gaussian 16 & Gauss View 06
ChemOffice Professional
Mnova Suite + CASE

Date: 03rd & 04th December, 2020 ~ Time: 10.00am onwards

Day 1 (03rd Dec 2020)

Gaussian 16 & Gauss View 06

Module 1: (2 Hrs)

Introduction of Gaussian 16

What is Gaussian 16? , Background of Electronic Structure Theory, Independent Particle Models, Model Chemistry, Basis Sets, Standard Basis Sets, SCF Convergence and Stability, Using ONIOM, Solvation, Periodic Boundary Conditions.

Module 2: (2 Hrs)

DFT Geometry & Frequency

What is DFT? Various Functions in DFT & Raman & IR frequency calculations. Geometry Optimization, Frequency, IRC, Scan calculations.

Module 3: (2 Hrs)

Introduction to GaussView 06 & Practical Considerations

Basics of Running Gaussian Calculations, Output Files, Anatomy of a Gaussian Input File, Gaussian Utility Programs, Computational, DFT Geometries and Frequencies, Summary of Standard Methods.

Day 2 (04th Dec 2020)

Session 1: ChemOffice Professional

Module 1: ChemDraw Professional (1 Hr)

- | | |
|------------------------------|----------------------------|
| ⦿ Basic Drawings in ChemDraw | ⦿ Templates |
| ⦿ Page Layout | ⦿ Preferences and Settings |
| ⦿ Shortcuts and HotKeys | ⦿ Drawing Biopolymers |
| ⦿ Drawing Monomer Sequences | ⦿ Structure=Name |
| ⦿ Advanced Drawing Tools | ⦿ ChemExcel/CombiChem |



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Module 2: Chem3D

(30 min)

Building a model and rotations, Generate 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.

Module 3: Signals NoteBook

(30 min)

Make notebook and experiments; share the experiments, chemical details, ChemDraw embedded notebook, working with MS Office in ELN and Reporting.

Session 2: Mnova Suite + CASE

Module 1: Mnova NMR

(30 min)

⦿ Basic Processing of 1D NMR

⦿ Basic Processing of 2D NMR

Module 2: Mnova MS

(30 min)

Basic MS Processing: TIC, Mass Spectra, CoAdd Peaks/Background Subtraction, MS Browser, UV Traces, Elemental Composition, Molecular Matching, Peak Purity, Reporting.

Module 3: Mnova Predict

(15 min)

Prediction of ¹H/¹³C/HSQC spectra from Structure and X Nuclei prediction

Module 4: Mnova CASE

(30 min)

1D and 2D spectral data importing, MCD, Structure constrain, Prediction of proposed structure

Workshop Speakers:

- ⦿ Mr. Charitra Gour
- ⦿ Dr. Sourab Sinha

Registration:

Registration is open for 50 participants, Register here: <https://forms.gle/JmyX7YQ6nSYv9T157> or Scan the QR Code

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