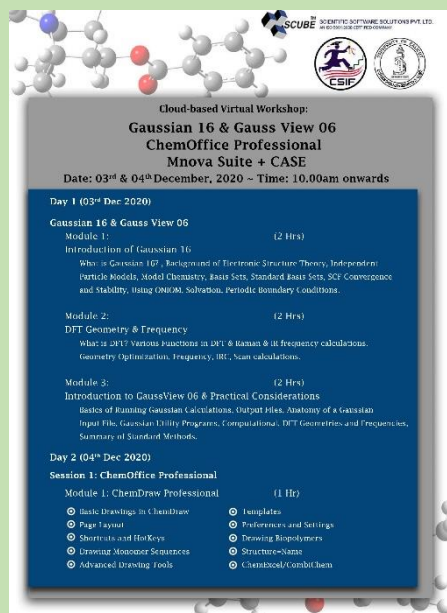


Cloud-based Virtual Workshop: Gaussian 16 & Gauss View 06 ChemOffice Professional Mnova Suite+CASE

Date: 03rd & 04th Dec 2020 ~ Time: 10:00 am Onwards



**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 to Gaussian 16
What is Gaussian (G), Background of Electronic Structure Theory, Introduction 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 functionals in DFT, 6-311g, 6-311g+it, frequency calculations, Geometry Optimization, Frequency, IR, NMR 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
Page Layout
Shortcuts and HotKeys
Drawing Molecular Structures
Advanced Drawing Tools
Templates
Preferences and Settings
Drawing Biopolymers
Structural-Units
Chemical/Combination



Module 2: Chem3D (30 min)
Building a model and rotations, Generate bond lengths/angles/dihedral angles, Trans is C is isomers, Steric energy of eclipsed and staggered conformers, Overlaying model to compare structural similarities, ROMD-DMD visualization, visualizing partial charge/dipole moments/van der Waals radius, Conformational Analysis, Molecular Dynamics, Stereochemistry.

Module 3: Signals Notebook (30 min)
Make notebook and experiments, share the experiments, chemical details, ChemView embedded notebook, working with MS Office in LMS 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, Cxid Peaks, Background Subtraction, MS Renamer, UV Traces, Elemental Composition, Molecular Weight, Peak Purity, Isotope.

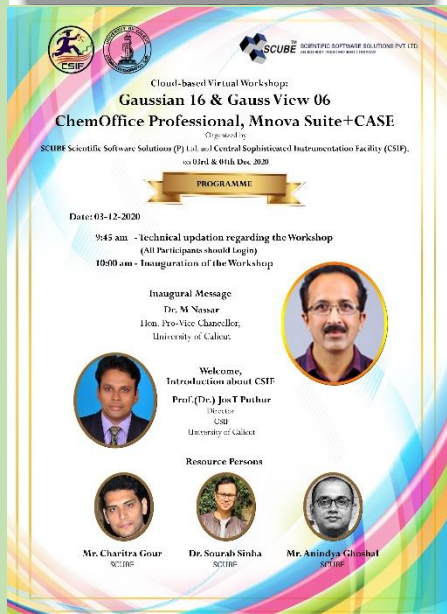
Module 3: Mnova Predict (15 min)
Prediction of ¹³C/¹⁵N/¹⁹F spectra from Structure and X-Ray prediction.

Module 4: Mnova CASE (30 min)
1D and 2D spectra data importing, MCD, Structure constraint, Prediction of proposed structure.

Workshop Speakers:
Mr. Charitra Gour
Dr. Sourabh Sinha

Registration:
Registration is open for 50 participants, Register here: <https://forms.gle/mvX7YQmSVy971L7> or Scan the QR Code

Requirement:
Central Sophisticated Instrumentation Facility (CSIF)
University of Calicut
Molepuzha-673035
Phone: 04942407400
Email: csiftechno@uoc.ac.in web: <https://csif.uoc.ac.in/>



**Cloud-based Virtual Workshop:
Gaussian 16 & Gauss View 06
ChemOffice Professional, Mnova Suite+CASE**
SCUBE Scientific Software Solutions (P) Ltd. and Central Sophisticated Instrumentation Facility (CSIF), on 03rd & 04th Dec, 2020

PROGRAMME
Date: 03-12-2020
9:45 am - Technical updation regarding the Workshop (All Participants should Login)
10:00 am - Inauguration of the Workshop

Inaugural Message:
Dr. M Nassar
Hon. Pro-Vice Chancellor,
University of Calicut

Welcome, Introduction about CSIF:
Prof. (Dr.) Jost Puthur
Director
CSIF
University of Calicut

Resource Persons
Mr. Charitra Gour
Dr. Sourabh Sinha
Mr. Anindya Ghoshal

The Two-day cloud based virtual workshop on Gaussian 16 & Gauss View 06, ChemOffice Professional, Mnova Suite+CASE was conducted on 03rd and 04th of December 2020. The event was organized by Central Sophisticated Instrumentation Facility (CSIF) in association with Scube Scientific Software Solutions Pvt Ltd.

The workshop could enlighten the participants in the field of Computational Chemistry and Biology. The workshop covered the full range of methods available in the Gaussian 16 package with emphasis on new methods and features which makes Gaussian 16 applicable to an ever-widening spectrum of research applications.

40 participants from various universities/research institutes participated in the Workshop.

Inauguration:

Dr. M Nassar

Hon'ble Pro-Vice Chancellor, University of Calicut

Workshop Speakers:

- Mr. Charitra Gour
- Dr. Sourabh Sinha
- Mr. Anindya Ghoshal