BON SECOURS COLLEGE
(AUTONOMOUS)

Vilar Bypass, Thanjavur – 613006

DEPARTMENT OF CHEMISTRY

organizes

Two-Day Virtual Workshop on Computational Chemistry

Modern Tools and Applications in Molecular Modeling and Simulation

Event Details

August 25 & 26, 2025

2.00 - 4.00 P.M.

Registration link
https://forms.gle/QejAjXM7t7yVaPGc7

Resource Person

Dr. NIVEDITA ACHARJEE
Associate Professor
Department of Chemistry,
Durgapur
Government College, West Bengal

Objectives of the event

- *Equipping with practical skills in applying computational chemistry tools to study selectivity, mechanisms, kinetics, and biological significance of chemical reactions.*
- *Utilizing the PASS Online Portal for predicting bioactivity of organic compounds and analyzing the results.*
- *Applying Avogadro software for regular teaching, learning, and research projects.*
- *Developing skills in conducting literature surveys of research articles and reviews to identify bioactive compounds.*
- *Training in Gaussian and GaussView software for: optimizing molecular structures, calculating Frontier Molecular Orbital (FMO) energies, exploring spectroscopic properties, and designing computational projects.*
- *Applying Multiwfn software to analyze electron density, molecular orbitals, and chemical reactivity descriptors.*
- *Using visualization tools such as UCSF-Chimera and Visual Molecular Dynamics (VMD) to study molecular structures and dynamics.*

Presided By
Rev. Sr. Dr. Victoria
Principal