Gaussian & ChemDraw Software Training

University of Delhi

9th August 2024

Gaussian Training (Session-1) Expending the limits of Computational Chemistry		
09 Aug Fri 10:00 a.m.	**Introduction to Gaussian & GaussView software** • **Background of DFT** • **Basis set selection**	**Bobby Solanki**
Assignment 1: Optimization of the compounds		
09 Aug Fri 11:00 a.m.	**Optimization of Chemical Structures** • How to draw Chemical structures in Gauss View • Making Gaussian Input: Single point calculations and optimization of Chemical Structure • Calculations and Analysis (HOMO-LUMO analysis, Energy Gap, Mullikan Charge, etc)	**Bobby Solanki**
Assignment 2: Transition state calculation		
09 Aug Fri 11:30 a.m.	**Transition state calculations and analysis Intermediate structure**	**Bobby Solanki**
Assignment 3: Spectroscopic calculations		

Solution Partner & Consultants:

PerkinElmer Informatics, USA *Gaussian Inc., USA* *Conflex Corp., Japan* *Fujitsu Biosciences, Poland* *CIMNE, Spain*
Mestrelab Research, Spain *Wolfram Research, USA* *Mackichan Inc., USA* *MIPAR Software Inc., USA* *Inte:ligand, Austria*

09 Aug Fri 12:00 p.m.	**Excited state and UV-Vis spectra calculation and Analysis** • Frequency and IR spectra calculations • VCD spectra calculations • NMR spectra calculation • TDDFT calculations • NBO Calculations and analysis	**Bobby Solanki**
09 Aug Fri 12:45 p.m.	**Q & A Session**	**Bobby Solanki**
09 Aug Fri 1:00 p.m.	**Lunch Break**	
ChemDraw Training (Session-2) **A Powerful Chemistry Communication Suite**		
09 Aug Fri 2:00 p.m.	• **Introduction of ChemDraw Software**	**Bobby Solanki**
Assignment 1: Working with ChemDraw		
09 Aug Fri 2:00 p.m.	• **Accurately represent organic, organometallic and polymeric and biopolymer materials.** • **Construct correct IUPAC names.** • **Calculate reaction stoichiometry.** • **Paste peptide, DNA and RNA sequences and have them interpreted chemically with sequence wrapping and shaping.** • **Generic structures** • **Highlight Colours** • **3D Cleanup** • **Shortcuts and Hotkeys** • **Conversion of Structure From 2D to 3D** • **Conversion of structure to Name and Conversion of Name to Structure** • **Prediction of 1H and 13C NMR Shifts** • **Save and copy as 3D Printable Format (.3MF)**	**Bobby Solanki**
Assignment 2: Working with Chem3D		
09 Aug Fri 3:00 p.m.	• **Visualize 2D molecules in 3D**	**Bobby Solanki**

	• Display properties like bond length, bond angles, dihedral angles and close contacts • Compute various properties with the help of computational engines associated in it	
Assignment 3: Working with ChemDraw/Excel		
09 Aug Fri 3:30 p.m.	• Add chemical structures, reactions, and other data from ChemDraw to an Excel worksheet • Build and manipulate structure • Calculate any of a vast array of chemical properties or examine search results from an SD file	**Bobby Solanki**
09 Aug Fri 4:00 p.m.	**Q & A Session**	**Bobby Solanki**