



# Vijay Bhaskar Mahajan

Email: [vijaymahajan2405@gmail.com](mailto:vijaymahajan2405@gmail.com)

Mobile: +917666182576

LinkedIn: [www.linkedin.com/in/vijay-mahajan-469512186/](https://www.linkedin.com/in/vijay-mahajan-469512186/)

## Professional Summary

A Computational chemist with an M.Sc. from ICT Mumbai and a strong foundation in computational chemistry and DFT calculations. Currently leveraging hands-on experience in multi-step synthesis, process development and optimization in an R&D environment. Seeking to apply this unique combination of predictive modelling and practical laboratory skills to solve complex challenges in early-phase API development, particularly in polymorph screening and reaction optimization.

## EXPERIENCE

### Senior Associate, Research & Development

Oriental Aromatics, Mumbai

July 2024 – Present

- **Project Leadership & Process Optimization:**
  - Independently planned, executed, and analysed all stages of complex organic syntheses at the laboratory scale.
  - Engineered and optimized reaction conditions (temperature, catalysts, solvent systems) to significantly improve product yield and purity, directly impacting project cost-effectiveness.
  - Authored and maintained comprehensive laboratory reports and documentation, ensuring seamless knowledge transfer to cross-functional teams for industrial scale-up efforts.
- **Analytical Troubleshooting & Problem-Solving:**
  - Utilized analytical techniques including TLC, GC, and GC-MS to meticulously monitor reaction progress, identify byproducts, and characterize final products.
  - Diagnosed and resolved critical process bottlenecks, such as inconsistent yields and impurity formation, by systematically analysing data and implementing targeted experimental solutions.
  - Conducted thorough literature reviews to integrate state-of-the-art synthetic methodologies and stay at the forefront of process development advancements.

## PROJECTS

### Master's Research Project-Computational Chemistry

Institute of Chemical Technology, Mumbai

July 2023-May 2024

- Investigated the nature of non-covalent interactions in binary mixtures of Solvated Ionic Liquids through a synergistic experimental and computational approach.
- Performed DFT and semiempirical QM calculations using Gaussian and GFN-xTB to model large molecular systems, correlating computational results with experimental Infrared Spectroscopy data to explain observed spectral shifts.
- This project provided a strong theoretical foundation for understanding the molecular quantum chemistry, principles of thermodynamics and intermolecular forces that govern solution-phase behaviour.
- Collaborated closely with experimental chemists, providing computational insights into electronic structure, reactivity, and vibrational spectra to help interpret their findings.

### Summer Research Intern- Computational Chemistry

Indian Institute of Technology, Palakkad

June – July 2023

Title: Computational studies on the hydrogenation of carbon dioxide to formic acid using a Mn-pincer complex in the presence of lysine.

- Conducted a comprehensive computational study on the hydrogenation of carbon dioxide to formic acid catalysed by a Mn-pincer complex.
- Executed a rigorous computational workflow, including geometry optimization of all reactants, intermediates, and transition states using the Gaussian quantum chemistry package.
- Performed detailed conformational analysis of key structures using the CREST utility and semiempirical GFN-xTB methods to ensure the lowest energy pathways were identified.
- Mapped the complete potential energy surface of the catalytic cycle, calculating activation barriers to elucidate the reaction mechanism and identify the rate-determining step.
- Gained significant hands-on experience performing complex calculations on high-performance computing (HPC) Linux clusters.

## TECHNICAL SKILLS

- **Computational Chemistry**
  - **Quantum Chemistry Packages:** Gaussian16, Orca, Psi4
  - **Software Familiarity & Training:** Schrödinger Suite (Maestro, Jaguar), COSMOtherm (Attended Workshop), AutoDock.
  - **Modeling Techniques:** DFT, Reaction Pathway & Transition State Analysis (IRC), Conformational Analysis (CREST), Molecular docking, Implicit/Explicit Solvation Models, TD-DFT for Excited States, Intermolecular Interaction Studies, Vibrational Spectroscopy.
  - **Analysis & Visualization:** GaussView6, VMD, Avogadro, ChemDraw, Origin Pro, PyMol
- **Laboratory & Process Chemistry**
  - **Synthetic Skills:** Multi-step Organic Synthesis, Process Optimization & Troubleshooting, Reaction Monitoring, Route Scouting, Laboratory Safety & Management.
  - **Analytical Techniques:** DSC, HPLC (academic), Gas Chromatography (GC), GC-Mass Spectrometry (GC-MS), Thin Layer Chromatography (TLC), Infrared Spectroscopy, NMR.
- **General & Programming**
  - **Operating Systems:** Windows, Linux
  - **Programming & Scripting:** Python
  - **Productivity Tools:** Microsoft Office, Notion, VS Code, Canva

EDUCATION

Degree	Institution	Year	CGPA/Percentage
M.Sc. (Chemistry)	Institute of Chemical Technology, Mumbai	2024	7.37/10
B.Sc. (Chemistry)	Fergusson College (Autonomous), Pune	2022	8.94/10
H.S.C.	D.R. Junior College, Nandurbar	2019	84.62%
S.S.C.	Ekalavya Vidyalaya, Nandurbar	2017	94%

SCHOLARSHIPS AND AWARDS

- DST-INSPIRE (SHE) Scholarship (2019-2024):** A prestigious scholarship awarded by the Department of Science and Technology, Government of India, for sustained academic excellence from Class 12 through Master's education.

COURSES AND CERTIFICATIONS:

- Introduction to Molecular Spectroscopy (Coursera)
- Python for Data Science and AI (IBM - Coursera)
- Data Science in Chemistry (Udemy)
- Python Complete Course for Beginners (Udemy)
- Machine learning specialisation-Deeplearning.ai-Coursera (Learning)
- Writings in Sciences (Stanford-Coursera)

LEADERSHIP & SCINETIFIC ENGANGEMENT

- Class Representative** - M.Sc. Chemistry, ICT Mumbai (2023-24):  
Acted as the primary liaison between a cohort of 25+ students and faculty, effectively communicating academic and administrative matters.
- Workshop Team Head** - Student Council of Chemistry (SCC-2024), ICT Mumbai:  
Conceptualized and managed academic workshops for Computational chemistry (CCB-24) students, enhancing peer-to-peer learning and engagement.
- PR Team Head** - Alchemy 2022, Fergusson College, Pune:  
Led public relations and outreach for the annual chemistry festival, significantly increasing event participation.