# MANADIP SUTRADHAR

+916033323244 sutradharmanadip01@gmail.com Linkedin GitHub

## Education

**Indian Institute of Technology Guwahati** **July 2023 – May 2025**
Master of Science in Chemistry, CPI: 7.93/10 Guwahati, Assam

**Maharaja Bir Bikram College** **June 2020 – May 2023**
Bachelor of Science in Chemistry, CGPA: 7.12/10 Agartala, Tripura

## Research Experience

**Effects of Microsolvation on Electron Attachment to the 5-Halogenated Uracil - Link**
Supervisor: Prof. Manabendra Sarma, IIT Guwahati, Master's Thesis

- Investigated the influence of halogen substitution and microsolvation on electron attachment to 5-halouracil at the B3LYP/aug-cc-pVDZ level of theory.
- Examined the stabilization of molecular orbitals and changes in electron affinities upon hydration at different positions of uracil, along with the effects of halogen substitution.
- Identified Br and I-substituted uracils as potential radiosensitizers due to enhanced electron affinity and dissociation tendencies. .

**Kinetic Study of Electron-Induced Reactions In Halogenated Guanine Base Pair 3´-dCMPH**
Supervisor: Prof. Manabendra Sarma, IIT Guwahati

- We investigated the electron affinity and the reactions induced by electrons generated during radiotherapy, using density functional theory (DFT) methods and a kinetic approach.
- The base pairing and the halogen substitution both enhance the electron capture ability of single nucleotide unit..
- Proton transfer from N1 of guanine to N3 of cytosine occur at near zero barrier after the electron attachment.
- Dehalogenation, a key process in radiosensitivity, was observed to be barrierless in the bromo and iodo analogs.
- **Manuscript submitted for publication** .

## Internship

**Machine Learning-Driven Molecular Property Prediction - Link** **May 2024 - July 2024**
Supervisor: Dr.Debashree Gosh, Indian Association for the Cultivation of Science Jadavpur, South kolkata

- Developed Machine Learning models (**Neural Networks, HistGradientBoosting, Multiple Linear Regression**) to predict molecular properties from SMILES strings, utilizing RDKit descriptors. .
- Conducted systematic **hyperparameter tuning** for Neural Networks by varying epochs and test sizes, and evaluated 41 regression algorithms using **LazyPredict** to identify optimal models.
- Compared the performance of differnent ML model across four distinct molecular properties and different molecular descriptors (Morgan and EState fingerprints), evaluating models using metrics such as **Mean Squared Error (MSE)** to identify best-fit solutions.

**Accenture Data Analytics & Visualization Virtual Internship - Link** **December-2023**

- performed data cleaning, modeling, and visualization to analyze content popularity.
- Delivered actionable insights and business recommendations through data storytelling and client-focused presentations.

## Personal Project

**Kaggle Competition: Stanford RNA 3D Folding - Link** **May-2025**

* Leveraged the Protenix model, a state-of-the-art deep learning architecture, to build an end-to-end pipeline for predicting the 3D atomic coordinates of RNA molecules directly from their nucleotide sequences.
* Configured the inference pipeline by setting model parameters (e.g., diffusion steps, number of cycles) and utilized Biopython and RDKit for data processing, achieving a public leaderboard score of 0.294 WRMSD out of approximately 18,386 submissions.

**NeurIPS Open Polymer Prediction 2025 (Kaggle Competition) - Link** **July-2025**

conducted by the University of Notre Dame

* Developed an end-to-end ML pipeline to predict five polymer properties (Tg, FFV, Tc, Density, Rg) using 200+ engineered features from SMILES, including RDKit molecular descriptors and graph-theoretic metrics
* Systematically benchmarked seven tree-based regressors (e.g., **CatBoost, XGBoost, and RandomForest**) using **Mean Absolute Error (MAE)** as the evaluation metric to identify the optimal model for each of the five target properties.
* Deployed a targeted prediction strategy using CatBoost Regressor for four properties (Tg, FFV, Tc, Density) and RandomForest Regressor for Rg, achieving MAE values of 35.87K, 0.007, 0.035, 0.039, and 1.81 Å respectively

## Technical Skills

**Programming Languages**: Python, Fortran. **Familiar**: C++
**Software**: Gaussian ,VMD, Jypyter Notebook,PyMOL.
**Data Analysis**: NumPy, Pandas, Matplotlib, Seaborn and Scikit-learn.
**Operating System**:Windows, Linux.

## Key Courses Taken

**Physical Chemistry**: Quantum Chemistry, Classical and Statistical Thermodynamics, Group Theory and Spectroscopy, Chemical Dynamics and Electrochemistry of solutions and interfaces, Applied Quantum Chemistry.
**Computational Chemistry**: Computers and Chemistry
**Organic Chemistry**:Organic Synthesis and Reactions, Reagents, Organic Reaction Mechanism
**InorganiChemistry**: Advanced transition metal and main group chemistry, Organometallic, Bio-Inorganic Chemistry

## Extracurricular Activities

**Student Mentorship**: Provided mentorship to first-year M.Sc. Chemistry students, offering academic support and personal guidance to help them navigate their coursework
**Subject Matter Expart at Course Hero**: Working as a Freelance Subject Matter Expert of Chemistry, Responsible for Providing Quality Solutions to Students on a Global Level.

## Achievements

**Secured All India Rank 316th in IIT JAM 2023**

## Certifications and Technical Courses

**Supervised Machine learning by Coursera - Link**
**Python for data science,AI and Development by coursera. - Link**
**Unsupervised Machine Learning by Coursera. - Link**
**Introduction to C++ by coding ninjas - Link**
**IIT Guwahati Summer Analytics 2024: Data Science and ML course - Link**