

Md Sahanawaz, PhD

Chemical Data Scientist · Lecturer

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PROFESSIONAL SUMMARY

Chemist, chemical data scientist and educator working at the intersection of chemistry, molecular information and machine learning. Research spans photochromic molecular sensing, multivariate spectroscopic analysis, cheminformatics and reproducible machine-learning workflows for chemical prediction and classification. Currently Lecturer and Head of the Department of Science & Humanities at Sheikhpara ARM Polytechnic.

EDUCATION

PhD in Chemistry — IISER Kolkata

2026 · Thesis: Photochromic Receptors for Nucleotide Detection Using Machine Learning Techniques

Azobenzene-based photochromic receptors combined with UV–Vis spectroscopy, PCA, LDA and supervised learning for nucleotide discrimination and chemical pattern recognition.

M.Sc. Organic Chemistry — Indian Institute of Technology Bombay

2018

B.Sc. Chemistry — Ramakrishna Mission Vivekananda Centenary College

2016

APPOINTMENTS

Lecturer & Head, Department of Science & Humanities

Sheikhpara ARM Polytechnic · Present (teaching since 2021)

- Teach Applied Chemistry, Applied Chemistry Laboratory and Fundamental Chemistry across Medical Laboratory Technology, Food Processing Technology and Computer Software Technology programmes.
- Faculty Coordinator, Institute Science Club — student engagement beyond the formal syllabus.
- Lead departmental academic coordination for Science & Humanities.

RESEARCH INTERESTS

- Cheminformatics — molecular descriptors, fingerprints, chemical-space and similarity analysis
- Machine learning for chemistry — classification, prediction, validation and interpretability
- Chemical sensing and pattern recognition — multivariate analysis of spectroscopic response patterns
- Molecular property prediction — descriptor/fingerprint-based predictive pipelines

SELECTED PUBLICATIONS

2025. A Smart Photoswitchable Sensor for Differential Detection of Multiple Nucleotides In Two Photoswitchable States using Machine Learning Techniques. *Analysis & Sensing*. DOI: [10.1002/anse.202500082](https://doi.org/10.1002/anse.202500082)

2024. Sequence effects on the thermal cis–trans isomerization of side-chain stearate-containing azobenzene polymers. *The Journal of Physical Organic Chemistry*. DOI: [10.1002/poc.4599](https://doi.org/10.1002/poc.4599)

2021. Photoswitchable Molecular Glue for Carbon Nanotubes Reversibly Controls Electronic Mobility with Light. *ACS Applied Electronic Materials*, 3, 309–315. DOI: [10.1021/acsaelm.0c00857](https://doi.org/10.1021/acsaelm.0c00857)

SELECTED PROJECTS & TOOLS

Chemical Machine-Learning Pipeline

Reproducible workflows from chemical datasets to molecular representations, modelling, validation and interpretation (Python, RDKit, scikit-learn). Ongoing.

Machine Learning for Analyte Detection

PCA/LDA and classification methods for multidimensional sensing data. Ongoing.

Spectra Autopilot

UV–Vis plotting tool for spectrophotometer file upload, preview, plot and export — spectraautopilot.streamlit.app

TCSPC AutoFit

TECHNICAL SKILLS

Programming: Python

Cheminformatics: RDKit, molecular descriptors & fingerprints, chemical-space analysis

Machine Learning: PCA, LDA, Random Forest, Bayesian methods, classification, clustering

Experimental: UV–visible spectroscopy, spectroscopic pattern analysis

Workflow: preprocessing, exploratory analysis, feature engineering, model validation, visualisation

CREDENTIALS & EXAMINATIONS

CSIR-NET (All India Rank 17) · GATE · JAM · WBPS · Menno Henselmans Personal Trainer Certification

BEYOND CHEMISTRY

Certified personal trainer with interest in evidence-based human performance, resistance training and applying scientific reasoning to training and nutrition.