

Ms. ANKITA NISHAD

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CAREER OBJECTIVE

I am driven to leverage my expertise in computer-aided drug design and computational chemistry to make significant contributions to drug discovery and development. By fostering collaboration between computational and experimental researchers, I aim to enhance translational research by integrating computational predictions with experimental validation. I am eager to expand my skill set and leverage cutting-edge computational techniques to drive innovation in pharmaceutical sciences, contribute to the development of novel therapeutics, and make a lasting impact on global health and patient care.

EDUCATION

National Institute of Pharmaceutical Research & Education (NIPER Guwahati) | MS (Pharm.) in Medicinal Chemistry | June 2021- June 2023

CGPA: 9.1 (First Class Honors)

- **Relevant coursework:** Basics of Drug Action, Drug Design, Structure and Function of Biomolecules, Stereochemistry and Drug Action, Spectral Analysis, Logic in Organic Synthesis, Separation Techniques, Synthetic Aspects of Process Chemistry, Natural Products Chemistry, Industrial Process and Scale-up Techniques, Biostatistics
- **Thesis:** *In Silico* Studies on Fungal CYP51 Enzyme to Decode Selectivity Mechanisms using Redox Potential, Molecular Dynamics Simulations, and QM/MM Calculations

University of Mumbai | B. Pharmacy | June 2017-May 2021

CGPA: 8.19 (First Class Honors)

- **Relevant coursework:** Pharmaceutics, Pharmacology, Medicinal Chemistry, Pharmacognosy, Microbiology, Biotechnology
- **Project:** A Systematic Survey on Effect of Pandemic on Health

WORK/ RESEARCH EXPERIENCE

Sai Life Sciences Pvt Ltd | Research Chemist (CADD) | July 2023 – Present

- Proficient in computational drug discovery, employing molecular modeling, docking, and dynamics simulations with industry-standard software
- Familiarity with ligand-based design, pharmacophore modeling, and ICH-M7 genotoxicity assessment
- Comprehensive experience from literature review to advanced computational analyses for drug development, with a proactive approach to learning and applying new methods to enhance research outcomes

SCHOLARSHIP / ACHIEVEMENT

- Qualified for national competitive exam GPAT & NIPER JEE
- Recipient of a stipend totalling Rs. 12,400/ month for a two-year master's program.
- Registered and licensed pharmacist

CONFERENCE PRESENTATIONS

- **Schrödinger India UGM - June 19–20, 2025 | Hyderabad, India**
Participated in user talks and technical sessions showcasing the application of computational molecular design in drug discovery; gained insights into the latest platform developments from Schrödinger like FEP+.
- **MultiCASE - April 11, 2025 | Ahmedabad, India**
Attended sessions focused on *in silico* risk assessment, predictive toxicology, QSAR approaches for pharma impurities, and regulatory updates relevant to chemical safety.
- DBT-sponsored workshop on Bioinformatics in Computational Biology, Software Applications in Drug Discovery at CSIR– NEIST, Jorhat
- The International workshop on “Advanced Drug Design and Medicinal Chemistry 2023” (ADDMC-2023)

SKILLS

Technical skill

- **Molecular Modeling and Molecular Dynamics Simulations:** Proficient in using Schrödinger and AMBER22 (specializing in metalloprotein simulations), AutoDock Vina, GROMACS and VMD
- **LBDD Tools:** Experienced with Cresset’s Flare and Spark, OpenEye
- **Quantum Chemical Calculations:** Skilled in Gaussian16
- **Machine Learning:** Competent in data mining using ORANGE software

- **Visualization and Analysis:** Expertise in Pymol, ChemDraw, and Biovia Discovery Studio
- **Preclinical Assessment:** Genotoxicity assessment (ICH-M7) using CaseUltra,
- **Programming and Scripting:** Working knowledge of the Linux operating system, and basics of Python and Bash scripting
- **Laboratory Techniques:** instrumentation handling such as UV-Vis Spectroscopy (Shimadzu) and FT-IR (Shimadzu)
- **Software Competence** - Microsoft Office Suite, Canva

Interpersonal Skills

- Leadership, Teamwork, Adaptability, Presentation skills, Communication
- **Openness to Learning:** Enthusiastic about acquiring new knowledge and tools required for innovative and interdisciplinary research

ADVANCED TRAINING / COURSES

- Data Science & Analytics course from HP LIFE and HP Foundation
- Data Visualization with Power BI course from Great Learning Academy
- Soft skill Development
- Microsoft Excel

CO-CURRICULAR ACTIVITIES

- Student Volunteer, "Sahay" Student NGO, NIPER Guwahati (2022-2023)
- Student Cell Social Media Editing Head, NIPER Guwahati (2022-2023)

REFERENCES

1. Dr Vaibhav Anil Dixit
Assistant Professor, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, Guwahati, Department of Pharmaceuticals, Ministry of Chemicals and Fertilizers, Govt. of India
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Supervisor for Masters project
2. Dr Kapileswar Seth
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