Dr. Anupama Sharma

Research Associate-I
R&D, International Institute of Information Technology, Telangana, Hyderabad
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Research Interest & Furture Research Prospect

- Multiscale Modeling and Simulation
- Molecular recognition and spectroscopy
- Forcefield parameterization and development in MD simulation techniques.
- Machine Learning
- My long-term goal is to develop advanced computational tools and multiscale modeling approaches to deepen our understanding of complex biomolecular systems. By integrating molecular-level insights with systems-level modeling, I aim to unravel the mechanisms of biological function and dysfunction, contributing to the rational design of therapeutics.

Education

2018-2024 — **Ph.D Computational Chemistry**
Department of Computational Sciences
Central University of Punjab, Bathinda, India
Thesis title : *"**Structure and Dynamics of Complex Liquids Inside Confined Environment.**"*
Supervisor : Dr. Sudip Chakraborty

2016 – 2018 — **M.Sc. Chemistry (Medicinal Chemistry)**
CGPA: 6.88/10
Central University of Punjab, Bathinda, India
Project title : *"In vitro and In silico study of Essential oil Components from Eucalyptus tereticornis as Antibacterial Agents."*
Supervisor : Dr. Vikas Jaitak

2013 – 2016 — **B.Sc.(Hons.) Chemistry**
68.59 % ,First Divison
Shyam lal college, University of Delhi, New Delhi, India.

Research Publications

5. Investigation into in silico and in vitro approaches for inhibitors targeting MCM10 in Leishmania donovani: a comprehensive study.
Saha, S., **Sharma, Anupama**, Bhowmik, D., & Kumar, D. (2024). Investigation into in silico and in vitro approaches for inhibitors targeting MCM10 in Leishmania donovani: a comprehensive study. Molecular Diversity, 1-16.

4. Influence of CTAB Reverse Micellar Confinement on Tetrahedral Structure of Liquid Water.
Anupama Sharma, M.anand, & Chakraborty, S. (2025). The Journal of Physical Chemistry B - jp-2024-04773p.R3

3. Integrating traditional QSAR and read-across-based regression models for predicting potential anti-leishmanial azole compounds.
Nandi, R., **Sharma, A.**, Priya, A., & Kumar, D. (2024). Integrating traditional QSAR and read-across-based regression models for predicting potential anti-leishmanial azole compounds. Molecular Diversity, 1-25.
2. Identification of molecular interactions of pesticides with keratinase for their potential to inhibit keratin biodegradation.
Gahatraj, I., Roy, R., **Sharma, A.**, Phukan, B. C., Kumar, S., Kumar, D., ... & Borah, A. (2024). Identification of molecular interactions of pesticides with keratinase for their potential to inhibit keratin biodegradation. In Silico Pharmacology, 12(1), 54.
1. Micro-Solvation of Propofol in Propylene Glycol-Water Binary Mixtures: Molecular Dynamics Simulation Studies.
Sharma, Anupama, Kumar, V., & Chakraborty, S. (2023). Micro-Solvation of Propofol in Propylene Glycol–Water Binary Mixtures: Molecular Dynamics Simulation Studies. The Journal of Physical Chemistry B, 127(51), 11011-11022.
Featured on the Cover Page of JPCB, Vol. - 127(51), (Dec, 28, 2023).

Online Courses Attended

Sep to Dec 2020 — **Basic Statistical Mechanics, Prof. Biman Bagchi, IIT Bombay, SWAYAM-NPTEL**

Oct 2021 to Jul 2022 — **Foundations of Modern Machine Learning conducted by** , IIIT Hyderabad.

Awards and Fellowship

- Doctral Fellowship by Council of Scientific and Industrial Research (CSIR) on the basis of National entrance test for Junior Research Fellow
  (CSIR-NET/JRF-2017,Dec) All India Rank in Chemical Sciences - 126
- Graduate Aptitude Test in Engineering (GATE-2018)
  Gate Score - 331
- Common University Entrance Test (CUCET(Ph.D.))-2018
- Common University Entrance Test (CUCET(Postgraduation))-2016

Skills

Languages	Proficiency in English and Hindi.
Operating system	Ubuntu, Windows, macOS.
Coding	**FORTRAN**, **Python**, Bash scripting, Tcl/Tk, AWK, and LaTeX.
Molecular Dynamics Simulation packages	Gromacs, AMBER, NAMD, CHARMM-GUI, Auto Dock Vina, Schrodinger
Qunatum Calculation Packages	Gaussian, psi4, Mulitwfn
Molecular modeling and Plotting tools	GaussView, Avogadro, VMD, Pymol, ChemDraw, Chimera, Xmgrace, gnuplot

Workshops and Confrences

CECAM Conference MD@60 - 2024 — Poster Presentation : Micro-solvation of Propofol in Propylene Glycol-Water Binary Mixture : Molecular Dynamics Simulation Studies.

Workshops and Confrences (continued)

TCB-2022, NIPER-Mohali	Poster Presentation : Effect of Confinement On Water Dynamics: Dependence of Temperature and Diameter of Carbon Conduits
TCS-2021, IISER-Kolkata	Poster Presentation "Differential Dynamics and Structural Investigation of a Propylene Glycol-Water Binary Solution from Microscopic View of Molecular Dynamic Simulation and Analysis."
Jan 20-24, 2020	Introduction to gaussian : Theory and practice, Hyderabad

References

Dr Sudip Chakraborty (Assistant Professor)
Central University of Punjab,India
sudip.chakraborty@cup.edu.in

Prof. U. Deva Priyakumar (Professor)
Centre Head, Center for Computational Natural Sciences and Bioinformatics (CCNSB)
International Institute of Information Technology (IIIT), Hyderabad
Academic Head, IHub-Data, Member Secretary, IIIT Hyderabad
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Diwakar Kumar (Assosciate Professor)
Assam University, Silchar, India
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Rakesh Srivastava (Assistant Professor)
Vellore Institute of Technology, Bhopal, India
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