

Dr. Anupama Sharma

Research Associate-I

R&D, International Institute of Information Technology, Telangana, Hyderabad

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🎓 <https://scholar.google.com/citations?user=Kvq6pisAAAAJ&hl=en>



Research Interest & Future 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 Division
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 Conferences (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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Dr. Diwakar Kumar (Associate Professor)

Assam University, Silchar, India

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Dr. Rakesh Srivastava (Assistant Professor)

Vellore Institute of Technology, Bhopal, India

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