

Akshatha

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EDUCATION

Indian Institute of Science, Bengaluru

Master of Technology, Computational and Data Science

(August 2023 - Ongoing)

CGPA: **8.40/10**

- **Courses:** Numerical Linear Algebra, Scalable Systems, Data Science, Random Variates in Computation, Numerical Methods, Applied Linear Algebra and Optimisation, Numerical Solutions of Differential Equations
- **Electives:** Bioinformatics, Statistical Thermodynamics, Advanced Methods in Molecular Simulations, Conformational and Structural Aspects of Biopolymers
- Awarded the Ministry of Education (MOE) fellowship for the programme

Manipal Institute of Technology, Manipal

Bachelor of Technology (Honours), Chemical Engineering

(June 2019 – June 2023)

CGPA: **9.79/10**

- Minor specialisation in Fundamentals of Computing (Python)
- Honours in Chemical Engineering (Numerical Methods, Optimisation & Advanced Control Theory)
- Gold medallist (Batch of 2019-23), Chemical Engineering
- Awarded the AICTE scholarship for the programme (AICTE Rank 1)

RESEARCH EXPERIENCE

Master's Dissertation

Optimisation of Fold-based Modular Force Field Parameters for Globular Proteins

(May 2024 – ongoing)

Biomolecular Computation Laboratory

Advisor: Dr Debnath Pal (Professor, Department of Computational and Data Sciences)

Bachelor's (Hons) Dissertation

(July 2022 – May 2023)

Applications of Deep Eutectic Solvents: Experimental Investigations and Atomistic Insights Using Molecular Dynamics Simulations

Advisor: Dr -Ing Anoop Kishore Vatti (Assistant Professor, Department of Chemical Engineering)

- Experimentally investigated the effects of synthesized DESs on asphaltene aggregation using FTIR and microscopy
- Simulated the effects of lysozyme structure and dynamics in various DESs using DESMOND
- Published two research papers reporting the findings of this work ([1](#),[2](#))
- Secured first position in paper presentation at *Chemignite 2023*, the Annual Department Symposium, and an institute-level seed funding of Rs. 10,000 for the project

Peptide-Solvent Interactions: Exploring Coordination Number as a Collective Variable to Characterise Peptide Hydrophobicity

Advanced Methods in Molecular Simulations Project

- Employed umbrella sampling using PLUMED with the GROMACS simulation engine to understand the relationship between solvent coordination number and the hydrophobic nature of various dipeptides

Project Cell-tinel

(February 2021 – November 2021)

Member, Research Subsystem, Manipal BioMachines ([Website](#))

- Researched and documented mechanisms and product implementation and came up with solutions for the selection of the bacterial chassis required for increased efficiency against stem borers in paddy
- Communicated with diverse stakeholders (scientists, industry representatives and farmers) at various stages of the project
- The interdisciplinary team presented the project at the international Genetically Engineered Machine (iGEM) Competition 2021 and won the bronze medal. The project also won the Impact Grant of \$2500 from the iGEM foundation

SKILLS

Programming: Python | C++ | Shell Scripting | MATLAB | LaTeX

Software: GROMACS | Schrödinger | Aspen Plus | AutoCAD

PUBLISHED LITERATURE

Hebbar, A., Debraj, D., Acharya, S. et al. (2023). Deep eutectic solvents interaction with asphaltenes: A combined experimental and molecular dynamics study, *Journal of Molecular Liquids*, 387, 10, <https://doi.org/10.1016/j.molliq.2023.122627>

Hebbar, A., Dey, P. & Vatti, A.K. (2023). Lysozyme stability in various deep eutectic solvents using molecular dynamics simulations, *Journal of Biomolecular Structure and Dynamics* 1-9, <https://doi.org/10.1080/07391102.2023.2275178>

Hebbar, A., Selvaraj, R., Vinayagam, S. et al. (2023). A critical review on the environmental applications of carbon dots. *Chemosphere*, 313. <https://doi.org/10.1016/j.chemosphere.2022.137308>

AWARDS

- Recipient of Dr PG Krishnamoorthy Memorial Award (2022) and Best Outgoing Student Award (2023)
- Received the Diamond Jubilee award for academic achievement three times in a row

EXTRA CURRICULARS

Indian Institute of Chemical Engineers, Manipal Chapter

(January 2021-December 2022)

Managing Committee Member (2021), Technical Head (2022)

- Organised guest lectures by industry professionals and academic researchers, as well as student interaction sessions on placements and higher education opportunities.
- Played a key role in coordinating Chemignite 2021, the annual department symposium as a Managing Committee member
- Acted as Master of Ceremonies (MC) for numerous seminars and technical events

Research Society, Manipal

(December 2021-December 2022)

Member, Biotechnology domain

- Collaborated with fellow student researchers and explored various research domains within biotechnology.
- Trained in research methodologies and academic writing and applied these skills to my domain of interest.

Violinist

- Secured 97.75% in the Karnataka Music Junior Grade Instrumental Examinations 2020
- 11 years of performances in showcases, competitions and festivals in various genres
- 1 year of experience as a violin tutor at Rhythmica Academy run by IISc's music club, Rhythmica
- Represented IISc at IICM 2023 held in IISER Mohali, secured silver medal in Battle of the Bands and bronze medal in Mehfil (Classical performance)