Akshatha

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EDUCATION

Indian Institute of Science, Bengaluru (Aug 2023 - Ongoing)
Master of Technology, Computational and Data Science *CGPA: **8.40**/10*

- Awarded the Ministry of Education (MOE) fellowship for the programme

Manipal Institute of Technology, Manipal (Jun 2019 – Jun 2023)
Bachelor of Technology (Honours), Chemical Engineering *CGPA: **9.79**/10*

- Minor specialisation in Fundamentals of Computing (Coursera)
- Gold medallist, recipient of Dr PG Krishnamoorthy Memorial Award (2022) and Best Outgoing Student Award (2023)
- Three-time winner, Diamond Jubilee Award (2020-2022)
- Awarded the AICTE scholarship for the programme

INTERNSHIPS

BASF India Limited, Mangalore Works (Jul 2022)
Intern, Dispersions Plant

- Gained insights into operations, planning and scheduling, safety, and process control, while developing skills in risk management, cost considerations, communication, and resource management through professional mentorship.
- The project titled **"Resource Conservation Using Pressure Reducing Valves (PRV)"** analysed utility consumption data with and without PRVs from the past 15 months. The use of PRVs cut average monthly expenditures on compressed air by 3 times, providing a return on investment in just 7 months

PROJECTS

M. Tech. Dissertation (May 2024 – ongoing)
Title: "Optimisation of Fold-based Modular Force Field Parameters for Globular Proteins"
Advisor: *Dr Debnath Pal, Professor, CDS (Biomolecular Computation Laboratory)*

- This project involves a detailed analysis of how various force fields model the behaviour of proteins, comparing model performance with experimental (NMR) data, and optimising force field parameters specific to protein folds

B. Tech. (Hons.) Dissertation (Jul 2022 – May 2023)
Title: "Applications of Deep Eutectic Solvents (DES): Experimental Investigations and Atomistic Insights Using Molecular Dynamics Simulations"
Advisor: *Dr -Ing Anoop Kishore Vatti, Assistant Professor, Department of Chemical Engineering*

- This study combined experimental and computational methods to investigate the impact of DESs as environmentally friendly solvents for studying asphaltene aggregation and as stabilising solvents for lysozyme
- Published two research papers discussing the results of this work [1, 2]
- Secured an institute-level seed funding of Rs. 10,000 for the project, and bagged the first position in paper presentation at the Chemignite 2023 department symposium

Project Cell-tinel (iGEM) (Feb 2021 – Nov 2021)
Title: Developing an Endophytic Biopesticide for the Treatment of Stem Borers in paddy
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++ | LaTeX | Shell scripting
Software: MATLAB | Schrödinger | GROMACS | Aspen Plus | AutoCAD | LabVIEW

PUBLICATIONS

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 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, R., Varadavenkatesan, T., Kumar, P. S., Duc, P. A., & Rangasamy, G. (2023). A critical review on the environmental applications of carbon dots. *Chemosphere*, *313*. https://doi.org/10.1016/j.chemosphere.2022.137308

Vinayagam, R., **Hebbar, A.**, Senthil Kumar, P., Rangasamy, G., Varadavenkatesan, T., Murugesan, G., Srivastava, S., Concepta Goveas, L., Manoj Kumar, N., & Selvaraj, R. (2023). Green synthesized cobalt oxide nanoparticles with photocatalytic activity towards dye removal. *Environmental Research*, *216*. https://doi.org/10.1016/j.envres.2022.114766

Pai, S., **Hebbar, A.**, & Selvaraj, S. (2022). A critical look at challenges and future scopes of bioactive compounds and their incorporations in the food, energy, and pharmaceutical sector. *Environmental Science and Pollution Research* 29(24) 35518–35541. https://doi.org/10.1007/s11356-022-19423-4

COURSEWORK AND COURSE PROJECTS

M.Tech.

- **Courses**: Numerical Linear Algebra, Introduction to Data Science, Scalable Systems, Random Variates in Computation, Numerical Methods, Applied Linear Algebra and Optimisation

- **Electives:** Bioinformatics, Statistical Thermodynamics, Advanced Methods in Molecular Simulations, Conformational and Structural Aspects of Biopolymers

Peptide-solvent interactions: exploring coordination number as collective variable to characterise peptide hydrophobicity
Advanced Methods in Molecular Simulations Term Project

- Employed advanced sampling techniques (umbrella sampling) to understand the relationship between solvent coordination number and the hydrophobic nature of various peptides

Implementations from scratch (MATLAB, C++, or Python)

- Polynomial regression methods, ODE solvers, numerical differentiation, and integration routines
- SVD image compression algorithm, Page Rank Algorithm using power iteration
- Hierarchical and k-means clustering and analysis of algorithms on county-wise cancer-risk dataset
- Dynamic programming for local and global sequence alignment of proteins and spelling corrections

B.Tech.

- **Hons. Courses:** Numerical Methods, Optimisation of Chemical Processes & Advanced Control Theory

- **Electives:** Bioinformatics, Bioinspired Designs in Engineering, Virtual Instrumentation, Introduction to Nanotechnology**,** Risk and Safety Management, Renewable Energy

EXTRA CURRICULARS

Indian Institute of Chemical Engineers, Manipal Chapter
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
- Coordinated and acted as Master of Ceremonies for ChemIgnite 2021, the annual department symposium as a Managing Committee member, contributing to its successful organization and execution.

Research Society Manipal (Dec 2021-Dec 2022)
Member, Biotechnology Domain