SHARATH B S, M.Sc., Ph.D.

Computational Chemistry · AI Drug Discovery · Bioinformatics

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Portfolio · LinkedIn

PROFESSIONAL SUMMARY

Computational Chemist specializing in cheminformatics, molecular modeling, computational biology, and AI-assisted drug discovery. Experienced in developing computational workflows, analyzing complex biological datasets, and applying scientific computing to accelerate research and decision-making. Proven expertise in scientific literature evaluation, technical writing, and interdisciplinary collaboration. Expanding expertise in agentic AI, large language models (LLMs), and retrieval-augmented generation (RAG) through the development of intelligent scientific applications for biological data analysis, workflow automation, and scientific knowledge management.

PROFESSIONAL EXPERIENCE

Research Scientist Dec 2025 – Present

UR Advanced Therapeutics (BioVaram) | Hyderabad, India

- Build computational pipelines for rational peptide design, improving structural-stability and function prediction to guide candidate selection.
- Deploy ML models for peptide property prediction, reducing sequence-design and screening cycle time.
- Design and optimize self-assembling and cell-penetrating peptides (CPPs) with advanced MD simulations to support biomaterial development.
- Multi-omics analysis for exosome characterization and biomarker prioritization.

Postdoctoral Researcher Feb 2024 – Mar 2025

Pharmacoinformatics Research Group, Universität Wien | Vienna, Austria

Project: Roche ROADS — In silico predictive & translational safety

- Preclinical data analysis in CDISC SEND format to support regulatory-ready translational safety analyses.
- Developed and deployed knowledge-based ML models to predict clinical outcomes and safety profiles from preclinical toxicity data.
- Collaborate with toxicologists to map off-target effects and toxicity endpoints, enabling data-driven decisions in drug development.

Postdoctoral Researcher Aug 2021 – Dec 2023

Soongsil University | Seoul, South Korea

Project: In silico quorum-sensing inhibitor screening using cheminformatics tools (NRF, South Korea)

- Engineered end-to-end cheminformatics pipelines for high-throughput virtual screening, accelerating lead discovery from large compound libraries.
- Automated data extraction, processing, and proteochemometric modeling with reproducible Python workflows.
- Applied ligand- and structure-based CADD to identify and prioritize high-confidence drug candidates.

Assistant Lecturer Oct 2020 – Jun 2021

Kuvempu University | Shivamogga, Karnataka, India

Fostered an engaging teaching environment and mentored students in establishing early research careers in biotechnology.

Scientific Manager Nov 2014 – Apr 2015

DiponEd BioIntelligence | Bengaluru, India

Managed R&D on biological formulations (PRP, PRFM) and stem-cell isolation, culture, and maintenance.

EDUCATION

Ph.D. in Biotechnology Feb 2019

Kuvempu University | Karnataka, India

Thesis: Drug target identification through dynamics of protein interaction network analysis using VEGF-induced monocytes

- Pathway modelling, network pharmacology, and power-graph analysis; molecular docking, MD simulation, and binding free-energy calculation; experimental validation of bottleneck proteins with small-molecule compounds.

M.Sc. in Biotechnology Jun 2014

Sahyadri Science College, Kuvempu University | Karnataka, India

Project: Phytosynthesis, characterization, and induced toxic effect of zinc nanoparticles on mitotic chromosomes of Allium cepa L.

- Nanoparticle characterization (UV-Vis, FTIR, AFM, HR-TEM) and cytotoxicity assessment on Allium cepa L. root tips.

B.Sc. in Chemistry, Biotechnology & Zoology Jun 2013

Sahyadri Science College, Kuvempu University | Karnataka, India

CERTIFICATIONS

- Machine Learning and Molecular AI — Uresearcher LLC (Nov 2021 – Jul 2022). ML/DL for drug discovery with hands-on capstone.
- Data Analysis for Genomics — HarvardX / edX (Apr 2023 – Jul 2023). Bioconductor, functional genomics case studies, and advanced Bioconductor with capstone.
- Version Control of a Python Project using Git — Coursera (Mar 2023).

TECHNICAL EXPERTISE

- **Computational & Molecular Modeling:** MD simulations (GROMACS, Amber); coarse-grained MD (martini); enhanced sampling (steered MD, umbrella sampling, replica exchange); membrane–protein MD; free-energy calculations (MM/GBSA, MM/PBSA); molecular docking; protein/peptide modeling; interaction analysis (PyMOL, ChimeraX, VMD).
- **Cheminformatics & Molecular AI:** Molecular descriptors/fingerprints (ECFP, MACCS, RDKit); pharmacophore & QSAR modeling.
- **Data Science & MLOps:** Scikit-learn, TensorFlow, PyTorch; feature engineering; dimensionality reduction (PCA, t-SNE, UMAP); model interpretability (SHAP). Strong interest in agentic AI and RAG for developing data-to-insight workflows in bioinformatics.
- **Systems Biology & Network Analysis:** Multi-omics analysis; functional/pathway enrichment analysis; PPI/DDI networks (Cytoscape, STRING/STICH database).
- **Omics Data Analysis Tools:** Bioconductor & it packages - SRA Toolkit, FastQC, MultiQC, Cutadapt, Trim Galore, STAR, Bowtie2, kallisto, RSEM, Samtools, Subread, DESeq2.
- **Programming & HPC:** Python, Bash, Git/GitHub; large-scale simulations on HPC clusters (SLURM, PBS); SSH/SCP for remote workflow management.

SELECTED PUBLICATIONS

Total: 27 publications · Citations: 314 · Full list: Google Scholar

1. Sharath B. S., Kandagalla S., Lee J.* Development of machine learning models based on molecular fingerprints for selectivity of novel small molecules against JAK2 protein. J. Comput. Chem. 2023 (IF 4.8). https://doi.org/10.1002/jcc.27103
2. Sharath B. S., Rimac H., Lee J.* In-silico screening of quorum sensing inhibitor candidates obtained by chemical similarity search. Molecules 2022 (IF 4.6). https://doi.org/10.3390/molecules27154887
3. Sharath B. S., Kandagalla S., Vikas H. M., Pavan Kumar G. S., Prabhakar B. T.*, Manjunatha H.* A systems biology approach to identify the key targets of curcumin and capsaicin that downregulate pro-inflammatory pathways in human monocytes. Comput. Biol. Chem. 2019 (IF 3.1). https://doi.org/10.1016/j.compbiolchem.2019.107162

4. Sharath B S, Shivananda Kandagalla, Pavan Gollapalli, Bharath B R, Triveni H, Manjunatha Hanumanthappa*. Topology of protein-protein interaction network and edge reduction co-efficiency in VEGF signaling of breast cancer. NetMAHIB, 2017. IF-2.0 https://doi.org/10.1007/s13721-017-0157-6

5. Kandagalla S.†, Sharath B. S.†, Rimac H.*, Grishina M., Manjunatha H.*, Potemkin V.* Computational insights into the binding mode of curcumin analogues against EP300 HAT domain as potent acetyltransferase inhibitors. J. Mol. Graph. Model. 2020 (†Equal contribution; IF 3.0). https://doi.org/10.1016/j.jmgm.2020.107756

6. Sharath B. S., Kandagalla S., Manjunatha H.* A network pharmacology approach to investigate the pharmacological effect of curcumin and capsaicin targets in cancer angiogenesis by module-based PPI network analysis. J. Proteins Proteomics 2019. https://doi.org/10.1007/s42485-019-00012-y

SELECTED CONFERENCES & WORKSHOPS

- International Conference on Biological Physics (ICBP 2023), Seoul, South Korea (Aug 14–18, 2023).
  Presented title: “Computational Approach to Predict Off-target Binding Profile for Virtual Small Molecule Screening in Rational Drug Designing.”
- Lecture Notes in Computer Science (LNCS): Advances in Bioinformatics and Computational Biology (BSB 2020).
  Presented title: “A systems biology driven approach to map the EP300 interactors using comprehensive protein interaction network.”
- 2023 Annual Conference of the Korean Society for Bioinformatics (BIOINFO 2023), Yeosu, South Korea (Nov 13–15, 2023).
- Hands-on Training in Genomics and Transcriptomics — jointly organized by The University of Trans-Disciplinary Health Sciences and Technology (TDU) and Bangalore Genomics Centre (BGC), Centre for Functional Genomics and Bioinformatics, Bengaluru, India.
- International Workshop on Computational Techniques for Wetlab Data Analysis (IWCWA), National College (Autonomous), Tiruchirappalli, India (Sep 22–24, 2015).

REFERENCES

Available upon request.