SHIVA SHANKAR S., Ph.D.

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PROFESSIONAL SUMMARY

Ph.D. researcher with 7+ years integrating molecular biology, protein engineering, and quantitative proteomics to solve complex protein challenges. Core expertise: molecular biology, and computational structure prediction (AlphaFold2, inverse folding), proteomics method development (XL-MS, PTM enrichment, DIA/SWATH), and protein expression/purification of difficult targets. Co-inventor of patented insulin therapeutics with 6 publications and proven successful engineering functional variants from insoluble proteins.

EDUCATION

Ph.D. in Biological Sciences
CSIR-National Chemical Laboratory (NCL), Pune, India | July 2017 - December2025
Thesis: Structural and functional characterization of Meteorin and Meteorin-like proteins
Advisor: Dr. Mahesh Kulkarni

M.Sc. in Biotechnology Bharathiar University, India | 2009

B.Sc. in Biotechnology Bharathiar University, India | 2007

RESEARCH EXPERIENCE

Senior Research Fellow / Project Associate | CSIR-National Chemical Laboratory, Pune
July 2017 - 2025

Project: Role of Meteorin and Meteorin-like proteins in cellular metabolism

- Conducted comprehensive structural analysis, expression, and purification of recombinant Meteorin and Meteorin-like proteins.
- Performed biophysical, biochemical characterization to elucidate protein function in metabolic pathways and developed targeted proteomics approach for Metrnl.
- Utilized *de novo* structure prediction to identify functional receptor-binding regions and high-risk missense variants.
- Integrated structure-guided and inverse-folding approaches with biophysical, biochemical, and cross-linking analyses to study functional mechanisms of mouse Meteorin-like protein in metabolic regulation.

Project: Development and Characterization of Glycation Resistant Insulin

- Engineered a glycation-resistant insulin proteoform incorporating *de novo* solubility-tag design and optimized expression constructs to improve yield and intended for anti-diabetic therapy.
- Designed and established a novel *in vitro* workflow to study insulin glycation mechanisms and modification profiles.
- Innovation: Co-invented a patented method for preparing glycation-resistant insulin polypeptides (WO 2024/194897 A1).
- Designed protocols that significantly enhanced the productivity and efficacy of the research process.
- Analyzed insulin modification using mass spectrometry approaches.

- Also, Contributed to the discovery of potential multi-target-directed ligands for SARS-CoV-2 main protease.

Project Assistant II | CSIR-National Chemical Laboratory, Pune
April 2013 - July 2017

Project: Structural characterization of Santalene synthase from Indian sandalwood.

- Executed the expression and purification of Santalene synthase, followed by extensive crystallization and biophysical characterization.

Junior Research Fellow | IISER-Pune
July 2010 - April 2013

Project: Synthesis and structural characterization of gamma and hybrid gamma peptides as HIV-1 fusion inhibitors.

- Synthesized and characterized peptide inhibitors specifically designed for anti-retroviral therapy.
- Investigated antimicrobial activity of self-assembling short hybrid gamma lipopeptides.

Project Trainee | National Institute of Immunology (NII), New Delhi
July 2009 - Dec 2009

- Cloned, expressed, and purified HisA, HisB, and HisC2 proteins involved in the histidine biosynthesis pathway of *Mycobacterium tuberculosis*.

TECHNICAL EXPERTISE

- **Molecular Biology:** Molecular cloning, site-directed mutagenesis, recombinant protein expression (prokaryotic and eukaryotic expression systems).
- **Cell Culture:** Mammalian cell culture, CRISPR-based knockout generation, immunofluorescence, cell-based assays.
- **Proteomics:** Bottom-up and top-down proteomics; untargeted and targeted workflows (DDA, DIA/SWATH, PRM); targeted assay development; immunoprecipitation; ELISA, Western blotting, chemical cross-linking and cross-linking mass spectrometry (XL-MS); MALDI, data analysis using Maxquant, Skyline, Fragpipe, Basic skills in R and Python.
- **Protein Purification:** Chromatography (affinity, ion-exchange, gel filtration), HPLC, FPLC (ÄKTA), inclusion body solubilization and refolding strategies.
- **Protein Engineering, Modeling & Data Analysis:** Structural analysis (AlphaFold2/ColabFold, RoseTTAFold), inverse folding and sequence design (ProteinMPNN), homology modeling (Modeller, Schrödinger Prime), molecular docking and molecular dynamics simulations (GROMACS, Desmond).
- **Biophysical Techniques:** Circular dichroism spectroscopy, SEC-MALS, dynamic light scattering, isothermal titration calorimetry, atomic force microscopy.
- **Crystallography:** Protein crystallization (hanging and sitting drop), robotic systems (Hamilton, Mosquito), X-ray diffraction.

PUBLICATIONS & PATENTS

1. Patents

Shankar, S.S*., Kulkarni, M.J., Banarjee, R., Jathar, S., Rajesh, S. "A glycation resistant insulin polypeptide and a method of preparing the same thereof." WO 2024/194897 A1. Issued Sep 26, 2024.

2. Peer-Reviewed Journal Articles (*First author and Co-corresponding author)

Rajesh, S., Jathar, S., Banarjee, R., Sharma, M., Palkar, S., **Shankar, S.S*.**, & Kulkarni, M.J. (2025). A simple freeze-thaw based method for efficient purification of recombinant human proinsulin from inclusion bodies. *Protein Expression and Purification*, 227: 106645.

Shankar, S.S*., Banarjee, R., Jathar, S.M., Rajesh, S., Ramasamy, S., & Kulkarni, M.J. (2023). *De novo* Structure Prediction of Meteorin and Meteorin-Like Protein for Identification of Domains, Functional Receptor Binding Regions, and Their High-Risk Missense Variants. *Journal of Biomolecular Structure and Dynamics,* 42(9): 4522-4536.

Pandya, V.K., **Shankar, S.S**., Sonwane, B.P., Rajesh, S., Rathore, R., et al. (2023). Mechanistic insights on anserine hydrolyzing activities of human carnosinases. *Biochimica et Biophysica Acta (BBA)-General Subjects,* 1867(3): 130290.

Joshi, R.S., Jagdale, S.S., Bansode, S.B., **Shankar, S.S**., et al. (2021). Discovery of potential multi-target-directed ligands by targeting host-specific SARS-CoV-2 structurally conserved main protease. *Journal of Biomolecular Structure and Dynamics,* 39(9): 3099-3114.

Srivastava, P.L., Daramwar, P.P., Krithika, R., Pandreka, A., **Shankar, S.S.,** & Thulasiram, H.V. (2015). Functional Characterization of Novel Sesquiterpene Synthases from Indian Sandalwood, Santalum album. *Scientific Reports,* 5: 10095.

Shankar, S.S*., Benke, S.N., Nagendra, N., Srivastava, P.L., Thulasiram, H.V., & Gopi, H.N. (2013). Self-Assembly to Function: Design, Synthesis, and Broad-Spectrum Antimicrobial Properties of Short Hybrid *E*-Vinylogous Lipopeptides*. Journal of Medicinal Chemistry,* 56(21): 8468-8474.

3. Manuscripts under preparation

Inverse Folding Design Enables Soluble Expression and Functional Activity of Mouse Meteorin-Like Protein. **Shankar, S. S***; Jathar, S; Sharma, M; Dole, A; Rajesh, S; Banarjee, R; Kulkarni, M. J.

Characterization of Glycation-Modified Insulin Glargine by Top-Down Mass Spectrometry
Jathar, S; Dole, A; Rajesh, S; **Shankar, S. S***;* Kulkarni, M. J.

AWARDS & ACHIEVEMENTS

- 3rd Prize, Basic Science Category: Chellaram Foundation Diabetes Research Award, 7th International Diabetes Summit, Pune (2023).
- Travel Award: 11th Annual Meeting of Proteomics Society of India (2019).
- CSIR Senior Research Fellowship: Awarded for Ph.D. program at CSIR-NCL (2017).
- GATE Qualified: Graduate Aptitude Test in Engineering in Biotechnology, Rank 862 (2016).
- Summer Research Fellow (2008) - Awarded by the Indian Academy of Sciences to work with scientists on research-oriented projects.

WORKSHOPS & PROFESSIONAL TRAINING (SELECTED)

- 73rd Conference on Mass Spectrometry and Allied Topics (ASMS), Baltimore, USA | June 1-5, 2025.
- 21st Annual US HUPO Conference, Philadelphia, USA | February 22-26, 2025.
- Advanced Proteomics Technologies Workshop & Conference, IIT Bombay, India | Feb 17-20, 2024.
- Monsoon Advanced Proteomics School (MAPS), IIT Bombay, India | June 25-26, 2023.
- 7th International Diabetes Summit, Chellaram Diabetes Institute, Pune, India | March 10-12, 2023.
- 24th Congress of the International Union of Crystallography (IUCR), India | August 21-28, 2017.

TEACHING & MENTORSHIP

- **Instructor for two CSIR Integrated Skill Initiative programs**: *Targeted Proteomics* (2022) and *Basic to Advanced Proteomics* (2021).
- **Mentorship:** Trained 8 project students and 4 Ph.D. students in molecular biology, protein purification, and proteomics workflows.

SCIENTIFIC PEER REVIEW

- Reviewed manuscripts for *Analytical Biochemistry* and *Protein Expression and Purification*

REFERENCES

- **Dr. Mahesh J. Kulkarni**
  Chair & Senior Scientist, Biochemical Sciences Division
  CSIR-National Chemical Laboratory (CSIR-NCL), Pune, India
  | Email: mj.kulkarni@ncl.res.in

- **Dr. Sureshkumar Ramasamy**
  Cellcraft AI LLC, USA, | Former Scientist, CSIR-NCL, Pune, India
  | Email: sureshxtal@gmail.com

- **Dr. Dharmaraja Allimuthu**
  Assistant Professor, Department of Chemistry,
  Indian Institute of Technology (IIT) - Kanpur
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- **Dr. Hosahudya N. Gopi**
  Professor, Peptide Chemistry Laboratory
  Indian Institute of Science Education and Research (IISER), Pune, India
  | Email: hn.gopi@iiserpune.ac.in