GOPUKRISHNAN R

SENIOR SCIENTIST (APPLICATIONS) - CADD | COMPUTATIONAL BIOLOGY

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PROFESSIONAL SUMMARY

Computational biology postgraduate with specialization in Computer-Aided Drug Design (CADD). Experienced with computational drug discovery workflows, molecular docking, molecular dynamics simulation, protein-ligand analysis and application support for scientific researchers. Research interests include peptide-based inhibitor design and potential therapeutic strategies in neurodegenerative disease contexts. Delivered more than 20 scientific sessions including workshops and invited talks.

PROFESSIONAL EXPERIENCE

Senior Scientist (Applications) - CADD | Zastra Innovations Pvt Ltd | Nov 2025 - Present

Develop and implement molecular docking, simulation and binding energy analysis workflows; provide technical application support and training; validate in-silico protocols; analyze protein-ligand interactions; and collaborate with multidisciplinary research teams.

RESEARCH PROJECTS

Rational Design of TP5-Derived Peptidic Inhibitors Targeting GSK3beta for Potential Neuroprotection in Alzheimer's Disease

Laboratory of Computational and Structural Biology, JCMR | Mar - Sep 2025

Computational research focused on the design of peptide-based inhibitors targeting GSK3beta, informed by the biological context of CDK5-P25 and tau-associated signalling.

Phytochemical Screening and Antioxidant Activities of Aqueous Extract of Mentha spicata

University of Kerala | Nov 2021 - Mar 2022

Investigation of phytochemical classes in spearmint aqueous extract and the broader topic of antioxidant activity.

EDUCATION

MSc Computational Biology & Bioinformatics (CADD Specialization) - University of Kerala, 2023-2025 | CGPA 9.5/10

BSc Biochemistry - University of Kerala, 2019-2022 | CGPA 8.03/10

Diploma in Medical Coding - Transorze Solutions, 2022-2023

CORE TOOLS AND COMPETENCIES

Molecular modelling and simulations: AutoDock, AMBER, NAMD, GROMACS, Glide, PyRx, HADDOCK, HDock, Schrodinger Suite, Discovery Studio, PyMOL, ChemDraw, Open Babel. Programming and analysis: Python, R, Perl, data analysis and sequence analysis.

SELECTED SCIENTIFIC ENGAGEMENTS

Jan 2026 - Exploring Inducible Binding Conformations Using Cresset's Flare; International Conference on AI for Genomics and Drug Discovery, Bharathiar University.

Oct 2025 - Case Scenarios of Evidence-Based Ayurvedic Approach; CME Programme, Government Ayurveda College, Thiruvananthapuram.

Jul 2025 - Responsible AI in Research & Academia; invited speaker, University of Kerala.

Mar 2025 - Hands-on Workshop on Bioinformatics Tools and Techniques; resource person, Mar Ivanios College.

PUBLICATIONS AND SCIENTIFIC ABSTRACTS

Smitha P., Gopu Krishnan R., Sunitha P. (2025). Identification of Active Principles in Belladonna for Migraine Treatment: An in-silico Approach. Proceedings of HOMOEOVISION 2025.

Published abstracts in the National Symposium on Chemical Biology and Drug Design (JCMR); INCD-2025 / 11th Symposium on Translational Cancer Research; and International Conference on AI for Genomics and Drug Discovery.

RECOGNITION

First Prize (Poster Presentation): Rational Design of Peptidic Inhibitors Against GSK3beta for the Treatment of Alzheimer's Disease - INCD-2025 and 11th Symposium on Translational Cancer Research, University of Kerala.