Dr. Krishna Kant Gupta

Computational Biologist | Assistant Professor in Bioinformatics | Former MK Bhan Fellow

biokkscience@gmail.com | +91-6268467956 | linkedin.com/in/krishnakant-gupta-1a962a1a | ORCID: 0000-0002-4703-6452 | Pune, India

PROFESSIONAL SUMMARY

Accomplished computational biologist and Assistant Professor with 8+ years of post-doctoral research excellence in structural bioinformatics, drug discovery, and host–pathogen biology. Author of 30+ peer-reviewed publications in high-impact international journals including Nature Biotechnology, Frontiers in Bioinformatics, and Journal of Biomolecular Structure & Dynamics. Proven track record in molecular docking, MD simulations, QSAR modelling, and deep learning for biological macromolecular systems. Awardee of the prestigious MK Bhan Young Scientist Fellowship (DBT, Govt. of India). Committed to delivering high-quality academic instruction, advancing curriculum pedagogy, and establishing a competitive, grant-funded research programme.

ACADEMIC & RESEARCH EXPERIENCE

Assistant Professor in Bioinformatics

10-08-2026 – Present

Rajiv Gandhi Institute of IT and Biotechnology, Bharati Vidyapeeth University, Pune

- Delivering core academic coursework in Bioinformatics, Machine Learning in Biology, and Database Management Systems to undergraduate and postgraduate students.
- Overseeing computational biology lab curricula, mentoring student theses, and coordinating research training workflows in macromolecular modelling and genomics.
- Initiating interdisciplinary grant proposals and expanding institutional collaborations in structural drug design and host–pathogen AI predictive modelling.

MK Bhan Young Scientist Fellow

Apr 2023 – Mar 2026

National Centre for Cell Science (NCCS), Pune, India

- Orchestrated high-impact computational structural biology research, delivering 4 peer-reviewed publications encompassing deep learning PPI interface prediction and CXCR4 receptor drug targeting.
- Constructed the HVIface deep learning pipeline — a sequence-based framework decoding human–virus protein–protein interaction interfaces — accepted in Frontiers in Bioinformatics (2026), establishing a novel antiviral drug discovery tool.
- Executed AutoDock and GROMACS-based MD simulations to identify and validate inhibitor candidates against cancer target eIF4E and wheat dwarf virus Rep protein, advancing 2 studies to in vitro validation.
- Developed host–pathogen computational pipelines integrating network pharmacology and structural docking, generating mechanistic insights into therapeutic interventions for infectious diseases.
- Co-authored a landmark community benchmark study published in Nature Biotechnology — optimising sequence-based deep learning models of gene regulation.

Research Scientist

Jun 2019 – Mar 2023

SASTRA University, Thanjavur, Tamil Nadu, India

- Directed 5+ large-scale research projects spanning virtual screening, QSAR, genomics, and network pharmacology — producing 10+ SCI-indexed publications over a 4-year tenure.
- Executed high-throughput virtual screening campaigns and QSAR analyses targeting neuroinflammatory disorders, fungal pathogens (Cryptococcus neoformans), and CXCR4-mediated renal fibrosis.
- Forged interdisciplinary collaborations by integrating proteomics, transcriptomics, and computational docking to uncover novel drug targets and biomarkers.
- Mentored postgraduate student research projects in bioinformatics and contributed to teaching computational biology coursework.

EDUCATION

PhD in Bioinformatics | Pondicherry University (2013 – 2018)

- *Thesis: Purification, characterization and inhibition of cold-active lipase from Acinetobacter Radioresistens PR8*

M.Sc. in Bioinformatics | Devi Ahilya University, Indore (2010 – 2012)

B.Sc. (Biotechnology) | Devi Ahilya University, Indore (2007 – 2010)

FELLOWSHIPS & NATIONAL QUALIFICATIONS

- Conferred the MK Bhan Young Scientist Fellowship (DBT, Govt. of India) — competitive national early-career distinction.
- Qualified CSIR-NET, DBT-JRF, GATE, TNSET, and SLET-NE across life sciences and bioinformatics disciplines.

TEACHING & MENTORSHIP

- Instructing undergraduate and postgraduate courses in Bioinformatics, DBMS, and Machine Learning at Bharati Vidyapeeth University.
- Guided 1 Doctoral student (Mr. G Senthil Kumar) and numerous postgraduate research trainees through thesis development and publications.
- Delivered lectures in bioinformatics, structural biology, genomics, and computational methods at SASTRA University (2019–2023).

TECHNICAL SKILLS & EXPERTISE

• **Programming & Scripting:** Python (PyTorch, Biopython, scikit-learn, Pandas, NumPy), R

• **Structural Bioinformatics:** AutoDock, AutoDock Vina, GROMACS, PyMOL, UCSF ChimeraX, BLAST, Clustal Omega

• **Computational Methods:** Molecular Docking, Molecular Dynamics (MD) Simulations, QSAR, Virtual Screening, Network Pharmacology

• **Machine Learning & AI:** Deep Learning (CNNs, Graph Neural Networks), Protein Language Models (ESM-2, ProtBERT), Gene Regulatory Networks

• **Wet Lab Techniques:** Protein Purification, SDS-PAGE, Zymography, Enzyme Characterisation (Lipase kinetics)

PUBLICATIONS (PEER-REVIEWED JOURNAL ARTICLES)

• Gupta KK, Monty, Sajeeth, Geetha, and Chauhan R (2026). HVIface: A Sequence-Based Deep Learning Framework for Decoding Human–Virus Protein–Protein Interaction Interfaces. Frontiers in Bioinformatics. (Accepted)

• Nagasubramanian K, Vincent P, Gupta KK, and Chandran SA (2026). Inhibitor screening identifies Entecavir as a promising candidate targeting human eIF4E to block cap-dependent translation in cancer: an integrated in silico and in vitro study. Journal of Computer-Aided Molecular Design, 40(1), 43. https://doi.org/10.1007/s10822-025-00759-1

• Senthil Kumar G, and Gupta KK (2026). Identification of Small Chemical Modulators Capable of Blocking Membrane-Embedded CXCR4 Receptor Activity. Future Journal of Pharmaceutical Sciences. (Accepted) https://doi.org/10.1186/s43094-025-00915-2

• Nagasubramanian K, et al. (2026). Identification and Characterisation of Small Molecule Inhibitors Targeting Wheat Dwarf Virus Replication Protein (Rep). Discover Plants. (Accepted) https://doi.org/10.1007/s44372-025-00257-6

• Gupta KK, et al. (2025). Network Pharmacology-Based Modelling and Mechanistic Evaluation of Kabasura Kudineer for Therapeutic Applications. IJPER. https://doi.org/10.5530/ijper.20256024

• Rafi AM, et al. (2024). A community effort to optimise sequence-based deep learning models of gene regulation. Nature Biotechnology. https://doi.org/10.1038/s41587-024-02414-w

• Chintaluri PG, et al. (2025). Network Pharmacological Evaluation and Mechanistic Insights into the Medicinal Potential of Cressa cretica. Journal of Biomolecular Structure & Dynamics. (Accepted) https://doi.org/10.1080/07391102.2025.2472403

• Nagasubramanian K, and Gupta KK (2023). Interactome analysis implicates class II transactivator (CIITA) in depression and other neuroinflammatory disorders. International Journal of Neuroscience. https://doi.org/10.1080/00207454.2023.2279502

• Rathore AS, Gupta KK, et al. (2023). Targeting BRF2: Structural and Computational Insights for Therapeutic Intervention. Journal of Biomolecular Structure & Dynamics. https://doi.org/10.1080/07391102.2023.2256884

• Sreekala A, et al. (2023). Identification of coastal pesticide pollutants as potent inhibitors of Bacillus pasteurii urease mediated calcium carbonate precipitation: a computational approach. Journal of Biomolecular Structure & Dynamics. https://doi.org/10.1080/07391102.2023.2252089

• Senthil Kumar G, et al. (2023). Identification of CXCR4 Inhibitors for Therapeutic Targeting of Renal Fibrosis Using Computational Approaches. Journal of Biomolecular Structure & Dynamics. https://doi.org/10.1080/07391102.2023.2246575

• Krishnan S, et al. (2023). Waste to drugs: identification of pyrolysis by-products as antifungal agents against Cryptococcus neoformans. Journal of Biomolecular Structure & Dynamics. https://doi.org/10.1080/07391102.2023.2188960

• Kishore N, and Gupta KK (2022). Identification of small molecule modulators of class II transactivator-I using computational approaches. Journal of Biomolecular Structure & Dynamics. https://doi.org/10.1080/07391102.2022.2133011

- Rathore AS, et al. (2023). In silico identification of a promising inhibitor of Fusarium oxysporum f. sp. Lycopersici, Secreted in Xylem 1 protein. Molecular Diversity. https://doi.org/10.1007/s11030-023-10613-x
- Agase DM, et al. (2021). Differential gene expression and co-regulated expression of genes in leukemia: an in-silico approach to identify potent biomarker. Journal of Applied and Natural Science. https://doi.org/10.31018/jans.v13i2.2650
- Khan AM, and Gupta KK (2020). A Review on Pharmacokinetics properties of antiretroviral drugs to treat HIV-1 infections. Current Computer-Aided Drug Design. https://doi.org/10.2174/1573409916666201006143007
- Gupta KK, and Singh SK (2019). Cdk5: A main culprit in neurodegeneration. International Journal of Neuroscience. https://doi.org/10.1080/00207454.2019.1645142
- Gupta KK, et al. (2019). Constitutive Inflammatory Cytokine Storm: A Major Threat to Human Health. Journal of Interferon & Cytokine Research. https://doi.org/10.1089/jir.2019.0085
- Gupta KK, et al. (2018). Purification, Characterisation of Alkaline Cold Active Lipase from Acinetobacter radioresistens PR8 and Development of a New Zymography Method for Lipase Detection. Protein & Peptide Letters. https://doi.org/10.2174/0929866525666180905113206
- Gupta KK, et al. (2018). Glucovanillin: A potent inhibitor of lipase from Acinetobacter radioresistens. Informatics in Medicine Unlocked. https://doi.org/10.1016/j.imu.2018.01.002
- Gupta KK, et al. (2017). Scale-up and inhibitory studies on productivity of lipase from Acinetobacter radioresistens PR8. Journal of Bioscience and Bioengineering. https://doi.org/10.1016/j.jbiosc.2017.03.005
- Gupta KK, et al. (2016). Molecular docking and simulation studies of gustatory receptor of Aedes aegypti: A potent drug target to distract host-seeking behaviour in mosquitoes. Journal of Vector Borne Diseases.
- Rao BS, et al. (2014). Alzheimer's Disease: An interactome of many diseases. Annals of Indian Academy of Neurology. https://doi.org/10.4103/0972-2327.128551
- Balaji SR, et al. (2014). Molecular Docking Studies of Wide Spectrum Targets in Staphylococcus aureus — An Aim towards Finding Potent Inhibitors. Advances in Tech Biology & Medicine. https://doi.org/10.4172/2379-1764.1000115
- Barh D, et al. (2013). Conserved host-pathogen PPIs: Globally conserved inter-species bacterial PPIs based conserved host–pathogen interactome derived novel target in C. pseudotuberculosis, C. diphtheriae, M. tuberculosis, C. ulcerans, Y. pestis, and E. coli targeted by Piper betel compounds. Integrative Biology. https://doi.org/10.1039/c2ib20206a
- Barh D, et al. (2013). Exoproteome and Secretome Derived Broad Spectrum Novel Drug and Vaccine Candidates in Vibrio cholerae Targeted by Piper betel Derived Compounds. PLoS ONE. https://doi.org/10.1371/journal.pone.0052773
- Barh D, et al. (2012). Identification of Biomarkers for Skin Cancer Using Integrative Omics Approaches. European Journal of Cancer. https://doi.org/10.1016/S0959-8049(12)72056-7
- Hollmann A, et al. (2012). Tight controlled expression and secretion of Lactobacillus brevis SlpA in Lactococcus lactis. Biotechnology Letters. https://doi.org/10.1007/s10529-012-0887-6

BOOK CHAPTERS, CONFERENCES & PREPRINTS

- Elakkiya E, and Gupta KK (2021). High-throughput sequencing technologies. In: Bioinformatics in rice research: Theories and techniques, pp. 283–304. Springer Singapore.
- Gupta KK, et al. (2016). Identification of Biomarkers and Molecular Signatures Associated with Myocardial Infarction. Precision Medicine in Cardiology.
- Nathan VK, et al. (2021). Ureolytic Biomineralization in Coastal Regions Inhibited by Pesticide Pollution: A Computational Approach. AFOB Malaysia Chapter International Symposium.
- Nandhakumar R, et al. (2022). Gene Expression Analysis of RNA-Seq Data from Human Osteoarthritis Knee. Research Square.
- Poorani R, et al. (2022). USAG1 protein as a drug target in teeth regeneration. bioRxiv.
- Sarveswari HB, et al. (2022). Development of a smart pH-responsive nano-polymer drug against Vibrio cholerae. Research Square.
- Elumalai E, et al. (2021). miRNA-based biomarker exploration in cervical cancer. bioRxiv.
- Swathika RS, et al. (2021). Peptide-based epitope design for SARS-CoV-2. bioRxiv.

SOFTWARE, ALGORITHMS & OPEN-SOURCE PROJECTS

• **HVIface (2026):** A sequence-based deep learning framework to predict and decode Human–Virus Protein–Protein Interaction interfaces (Frontiers in Bioinformatics, 2026).

• **DREAM Challenge (2024):** Benchmarked and optimised sequence-based deep learning models for gene regulation, contributing to community efforts published in Nature Biotechnology.

• **SCPred (2022):** Convolutional neural network (CNN) model for skin cancer detection and clinical image classification. github.com/KrishnaKantGupta123/SCPRED

PROFESSIONAL REFERENCES

- **Dr Krishna Ramadas —** Associate Professor (PhD Guide), Centre for Bioinformatics, Pondicherry University | Email: *ramadaskr@gmail.com*
- **Dr Radha Chauhan —** Scientist 'F' and MK Bhan Fellowship Mentor, National Centre for Cell Science (NCCS), Pune | Email: *radha.chauhan@nccs.res.in*
- **Dr Shekhar C Mande —** Distinguished Scientist & Honorary Professor, NCCS Pune & Savitribai Phule Pune University | Email: *shekhar.mande@gmail.com*
- **Dr Basant Kumar Tiwary —** Professor, Centre for Bioinformatics, Pondicherry University | Email: *basant68@gmail.com*
- **Dr Anshul Nigam —** Senior Assistant Professor, Amity University, Mumbai | Email: *anshulnigam2006@gmail.com*