NAGA RAJIV LAKKANIGA, PhD

Assistant Professor
Department of Chemistry and Chemical Biology
Indian Institute of Technology (IIT), Dhanbad, India.

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Work experience

***Indian Institute of Technology (Indian School of Mines)**, Dhanbad, Jharkhand, India* — *Jan'22- Present*

- **Assistant Professor**, Department of Chemistry and Chemical Biology
- Established **Drug Discovery Research Lab**
- Supervisor of 6 PhD theses (ongoing) and 11 Masters dissertations (completed)
- **Faculty In-charge** of internships and placements of M.Tech Pharmaceutical Science & Engineering

***Scripps Research Institute**, La Jolla, California, USA* — *Feb'21- Dec'21*

- Post-doctoral Associate
- Project: In-vitro assay development and discovery of novel small molecule inhibitors against various proteins involved in SARS-CoV-2 and influenza viruses.

***Wayne State University**, Detroit, USA* — *July'20-Feb'21*

- Visiting research fellow
- Project: Targeting KRAS pathway for anti-cancer drug discovery

***Cognizant Technology Solutions**, Coimbatore, Tamil Nadu, India* — *Sep'11-Aug'13*

- Programmer analyst

Education

PhD in Pharmaceutical Sciences — *Aug'16-July'20*

- **University of Arkansas for Medical Sciences, Little Rock, Arkansas, USA**
- Specialization: Oncology drug discovery
- Thesis title: Targeting Aurora Kinase B for cancer therapy: Molecular dynamics studies and discovery of selective first-in-class inhibitors

Master of Pharmacy — *Aug'14 - July'16*

- **Birla Institute of Technology and Science (BITS) Pilani, India**
- Specialization: Pharmaceutical Chemistry
- GPA: 9.11/10
- Dissertation: Design, molecular docking and molecular dynamics studies of a novel chemical scaffold as Cathepsin D inhibitors

Bachelor of Pharmacy (Honours) — *Aug'07 - July'11*

- **Birla Institute of Technology and Science (BITS) Pilani, India**
- GPA: 7.17/10
- Dissertation: Synthesis and Anti-Bacterial Activity Profile of Cyclized Diazonium Compounds

***Board of Intermediate Education,** Andhra Pradesh (12^{th})* — *July'05 – April'07*

- Group: Maths, Physics, Chemistry
- Percentage: 92.4 %

***Board of Secondary Education,** Andhra Pradesh (10^{th})* — *April'05*

- Percentage: 93.8 %

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Sponsored research projects

- Design, synthesis and biological evaluation of Monopolar spindle 1 inhibitors as potential therapeutics for triple negative breast cancer *Sep'22 – Sep'24*
    - Role: PI
    - Funding agency: Science and Engineering Research Board (SERB)
    - Amount: Rs. 31,79,000
- Synthesis and biological evaluation of novel small molecule inhibitors of Aurora Kinase B for various malignancies *Aug'22 –Aug'25*
    - Role: PI
    - Funding Agency: IIT (ISM) Dhanbad
    - Amount: Rs. 15,00,000
- Bioscopy - Towards modern transdisciplinary education and research in microscopy
    - Role: Co-PI
    - Funding Agency: University Grants Commission (UGC)
    - Amount: Rs. 1,14,66,000

Research interests

- Discovery and optimization of novel small molecule inhibitors of protein targets in various cancers
    - Current research focuses on RET mutations, Mps1 Kinase, USP1 and Ferroptosis pathways
- Medicinal chemistry of anti-viral drugs, particularly targeting influenza
- Computational structural biology: characterizing the unresolved protein conformations and allosteric sites
- Bioinformatics study of cancer databases for identification and validation of novel drug targets
- Development of generative AI platforms for pharmacokinetic properties assessment of small molecules

Teaching

- Principles of Pharmacology
- Clinical trials & Regulatory affairs
- Chemistry of Drug Design & Drug Action

Achievements and academic outreach

- Identified the first non-competitive Aurora B Kinase inhibitor, SP-96 (CAS No. 2682114-54-9)
- Reviewer for several journals in biomedical research, including,
    - Medicinal Research Reviews (IF: 10.9)
    - RSC Medicinal Chemistry (IF: 4.1)
    - Biotechnology and Applied Biochemistry (IF: 3.2)
    - Elsevier Bioorganic and Medicinal Chemistry (IF: 3.3)
    - The AAPS Journal (IF: 4.1)
- Delivered an invited talk in 27th ISCB International Conference (ISCBC-2022) entitled "Research and Innovation in Chemical, Pharmaceutical, and Biological Sciences" at BIT-Mesra Ranchi, Jharkhand in November, 2022.
- Delivered an invited talk and served as session chair in the "International conference on Challenges and Advancements in the Treatment of Neurological Disorders" held at Birla Institute of Technology & Science (BITS), Pilani, Rajasthan in March 2025.

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- First prize for Outstanding poster presentation at Drug Discovery and Development Colloquium, 2019
- All India Rank 355 in Graduate Pharmacy Aptitude Test (GPAT-2014), India with a percentile >99%
- All India Rank 338 in National Institute of Pharmaceutical Education and Research - Joint Entrance Examination (NIPER-JEE), 2014

Publications

From IIT (ISM) Dhanbad

Published

1) Singh, A., Lakkaniga, N.R. Exploring the Conformational Space of MPS1 Kinase Using Metadynamics. Proteins: Structure, Function, and Bioinformatics, 2025; 93: 1118-1127.
2) Halder, P., Rai, A., Talukdar, V., Das, P. and Lakkaniga, N.R., 2024. Pyrazolopyridine-based kinase inhibitors for anti-cancer targeted therapy. RSC Medicinal Chemistry, 15(5), pp.1452-1470.
3) Chatterjee, A., Jayaprakasan, M., Chakrabarty, A.K., Lakkaniga, N.R., Bhatt, B.N., Banerjee, D., Narwaria, A., Katiyar, C.K. and Dubey, S.K., 2024. Comprehensive insights into rheumatoid arthritis: Pathophysiology, current therapies and herbal alternatives for effective disease management. Phytotherapy Research, 38, 2764–2799.
4) Lakkaniga, N.R., Wang, Z., Xiao, Y., Kharbanda, A., Lan, L. and Li, H.Y., 2024. Revisiting Aurora Kinase B: A promising therapeutic target for cancer therapy. Medicinal Research Reviews, 44(2), pp.686-706.
5) Sharma, A., Jadhav, H.R., Rai, A., Lakkaniga, N.R., Chandramoorthy, H.C., Kamli, H.M., Alshahrani, M.Y. and Rajagopalan, P., 2024. A Comprehensive Review of Systemic Targeted Therapies in Cancer Treatment. Current Cancer Therapy Reviews, 20(5), pp.461-480.
6) Acharya, B., Saha, D., Armstrong, D., Hanafi, M., Herrera-Rueda, A., Lakkaniga, N.R. and Frett, B., 2024. Kinase inhibitor macrocycles: a perspective on limiting conformational flexibility when targeting the kinome with small molecules. RSC Medicinal Chemistry, 15(2), pp.399-415.
7) Sharma, P.D., Rallapalli, S. and Lakkaniga, N.R., 2023. An innovative approach for predicting pandemic hotspots in complex wastewater networks using graph theory coupled with fuzzy logic. Stochastic Environmental Research and Risk Assessment, 37(9), pp.3639-3656.
8) Acharya, B., Saha, D., Armstrong, D., Lakkaniga, N.R. and Frett, B., 2022. FLT3 inhibitors for acute myeloid leukemia: successes, defeats, and emerging paradigms. RSC Medicinal Chemistry, 13(7), pp.798-816.
9) Dorandish, S., Bhayekar, K., Singh, A., Kushwaha, N.D., Malin, E., Serafimovski, S., Kelm, J.M., Gavande, N., Lakkaniga, N.R. Evolution of Structure-guided Drug Design Strategies Targeting Mutations in Codon 12 of KRAS. RSC Medicinal Chemistry, 2025, 16, pp. 3429-3455.

From previous experience

10) Zhang, L., Moccia, M., Briggs, D.C., Bharate, J.B., Lakkaniga, N.R., Knowles, P., Yan, W., Tran, P., Kharbanda, A., Wang, X. and Leung, Y.K., 2022. Discovery of N-Trisubstituted Pyrimidine Derivatives as Type I RET and RET Gatekeeper Mutant Inhibitors with a Novel Kinase Binding Pose. Journal of Medicinal Chemistry, 65(2), pp.1536-1551
11) Lakkaniga, N. R., Zhang, L., Belachew, B., Gunaganti, N., Frett, B., & Li, H. Discovery of SP-96, the first non-ATP-competitive Aurora Kinase B inhibitor, for a reduced myelosuppression profile. European Journal of Medicinal Chemistry 2020, 203, 112589.
12) Lakkaniga, N. R., Gunaganti, N., Zhang, L., Belachew, B., Frett, B., & Li, H. Pyrrolo[2,3-d]pyrimidine derivatives as inhibitors of RET: Design, synthesis and biological evaluation. European Journal of Medicinal Chemistry 2020, 206, 112691.

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13) Lakkaniga, N. R.; Balasubramaniam, M.; Zhang, S.; Frett, B.; Li, H.-Y. Structural Characterization of the Aurora Kinase B "DFG-Flip" Using Metadynamics. The AAPS Journal 2019, 22 (1).
14) Balasubramaniam, M.*, Lakkaniga, N.R.*, Dera, A., Fayi, M.A., Abohashrh, M., Ahmad, I., Chandramoorthy, H.C., Rajagopalan, P. FCX-146, a potent allosteric inhibitor of Akt Kinase in cancer cells: Lead optimization of the second-generation arylidene indanone scaffold. Biotechnology and Applied Biochemistry. DOI: 10.1002/bab.1896
15) Zhang, L., Lakkaniga, N.R., Bharate, J., Wang, Xuiqi., … Li, H.Y. Discovery of Imidazo[1,2-a]pyridine- thiophene Derivatives as FLT3 mutants Inhibitors for Acute Myeloid Leukemia Through Structure-Based Optimization of an NEK2 inhibitor. European Journal of Medicinal Chemistry 2021, 225, 113776.
16) Moccia, M., Yang, D., Lakkaniga, N. R., Frett, B., ...& Carlomagno, F. Targeted activity of the small molecule kinase inhibitor Pz-1 towards RET and TRK kinases. Scientific Reports (2021) 11:16103
17) Moccia, M., Frett, B., Zhang, L., Lakkaniga, N. R., Briggs, D., Chauhan, R., Brescia, A., Federico, G., Santoro, M., McDonald, N., Li, H., Carlomagno, F. Bioisosteric discovery of NPA101.3, a second generation RET/VEGFR2 inhibitor optimized for single-agent polypharmacology. Journal of medicinal chemistry, 2020, 63, 4506-4516.
18) Naresh, G., Lakkaniga, N.R., Kharbanda, A., Yan, W., Frett, B. and Li, H.Y. Use of Imidazo [1, 2-a] pyridine as a Carbonyl Surrogate in a Mannich-Like, Catalyst Free, One-Pot Reaction. European Journal of Organic Chemistry, 2019(4), pp.770-777.
19) Saha, D., Kharbanda, A., Yan, W., Lakkaniga, N.R., Frett, B. and Li, H.Y., 2019. The Exploration of Chirality for Improved Druggability within the Human Kinome. Journal of medicinal chemistry, 2020, 63, 2, 441- 469
20) Gunaganti, N., Kharbanda, A., Lakkaniga, N. R., Zhang, L., Cooper, R., Li, H. Y., & Frett, B. (2018). Catalyst free, C-3 functionalization of imidazo [1, 2-a] pyridines to rapidly access new chemical space for drug discovery efforts. Chemical communications, 54(92), 12954-12957
21) Yan, W., Lakkaniga, N.R., Carlomagno, F., Santoro, M., McDonald, N.Q., Lv, F., Gunaganti, N., Frett, B. and Li, H.Y., 2018. Insights into current tropomyosin receptor kinase (TRK) inhibitors: development and clinical application. Journal of medicinal chemistry, 62(4), pp.1731-1760
22) Bharate, J. B., McConnell, N., Naresh, G., Zhang, L., Lakkaniga, N. R., Ding, L., ... & Li, H. Y. (2018). Rational Design, Synthesis and Biological Evaluation of Pyrimidine-4, 6-diamine derivatives as Type-II inhibitors of FLT3 Selective Against c-KIT. Scientific reports, 8(1), 3722
23) Krishna, H., Agarwal, A., Chamola, V., Lakkaniga, N.R., Hassija, V., Sikdar, B. (2021). A Review on the Role of Machine Learning in Enabling IoT Based Healthcare Applications. IEEE Access, 9, 38859-38890
24) Saha, D., Ryan, K., Lakkaniga, N.R., Smith, E.L., Frett., B. Pyrazoloadenines as Inhibitors for the RET Lung Cancer Oncoprotein Discovered via a Phenotypic Fragment-Based Approach. ChemMedChem 16 (10), 1605-1608
25) Rohmetra, H., Raghunath, N., Narang, P., Chamola, V., Lakkaniga, N.R.*, AI-enabled remote monitoring of vital signs for COVID-19: Methods, Prospects and Challenges. Computing (2021): 1-27.
26) Saha, D., Ryan, K., Lakkaniga, N.R., Acharya, B., Garcia, N.,… Frett, B. Targeting rearranged during transfection (RET) in Cancer: Small molecule inhibitors and their clinical development. Journal of medicinal chemistry 2021, 64 (16), 11747-11773
27) Bowraju, S.K., Penthala, N., Lakkaniga, N.R., … Crooks, P.A. Novel deoxyvasicinone-clioquinols as anticholinesterase therapeutics for Alzheimer's disease. Bioorganic and Medicinal Chemistry 2021, 45, 116311