

Publications

- 1) Singh, A., Lakkaniga, N.R. Exploring the Conformational Space of MPS1 Kinase Using Metadynamics. *Proteins: Structure, Function, and Bioinformatics*, 2025; 93: 1118-1127. DOI: 10.1002/prot.26796
- 2) 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.
- 3) 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.
- 4) 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.
- 5) 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.
- 6) 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.
- 7) 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.
- 8) 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.
- 9) 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.
- 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.
- 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).

Publications

- 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

Publications

- 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