Dr. D.Y. Patil Vidyapeeth's
Dr. D. Y. Patil Biotechnology & Bioinformatics Institute
Mumbai- Bangalore High way, Tathawade, Pune 411 033
Mail: info.biotech@dpu.edu.in, **Website:** www.biotech.dpu.edu.in

Mr. KIRAN BHARAT LOKHANDE

Designation : **Senior Research Fellow**

Email ID : **kiran.lokhande@dpu.edu.in**

Phone Number : **020-67919444 Extn. -9435**

Qualification : **M.S. Pharm. (Pharmacoinformatics)**

Area of interest : **Bioinformatics, Drug design, Molecular modeling, docking, dynamics, QSAR studies of Cancer Proteins**

Academic Qualifications:

M.S. Pharmacy (2014-2016) - National Institute of Pharmaceutical Education and Research (NIPER), Hajipur, Bihar, India.

B. Pharmacy (2010-2014) – University of Solapur, Solapur, India.

Professional Experience:

- **ICMR | Senior Research Fellow (ICMR-SRF) |** Bioinformatics Research Laboratory, Dr. D.Y. Patil Biotechnology and Bioinformatics Institute (June 2019 – Present).
- **DST-SERB | Senior Research Fellow (DST-SERB SRF) |** Bioinformatics Research Laboratory, Dr. D.Y. Patil Biotechnology and Bioinformatics Institute (Dec. 2018 – June 2019).
- **DST-SERB | Junior Research Fellow (DST-SERB JRF) |** Bioinformatics Research Laboratory, Dr. D.Y. Patil Biotechnology and Bioinformatics Institute (Oct. 2016 – Nov. 2018).
- **Project: "*Molecular modeling and docking studies on Deguelin and its derivatives with cell cycle arrest, apoptosis and anti-angiogenesis pathway proteins in cancer cell signaling pathway*",** funded by DST-SERB, New Delhi
- **Principal Investigator**: **Dr. K. Venkateswara. Swamy**, Associate Professor, Bioinformatics Research Laboratory

Professional Membership:

1) Life-Time Member: Institute of Scholars (InSc), India.

Reviewer:

1) Journal of Bimolecular Structure and Dynamics, Taylor & Francis.
2) InSc- International Journal of Basic and Applied Sciences.

Projects Undertaken:

1) Worked and submitted an academic project on, **"Discovery of novel GPR3 inhibitors using structure based and ligand based approaches".** During the course of M.S. Pharmacy (2014-2016), NIPER, Hajipur, India.
2) Worked and submitted an academic project on, **"Biodegradable Polymer as Drug Delivery System",** during the course of T.Y. B. Pharmacy (2012-2013), College of Pharmacy Akluj, university of Solapur, Solapur, India.

Computer Skills:

1) **Operating System:** Window, Ubuntu, Linux
2) **Languages:** JAVA, C++, Python, R, Perl
3) **Database:** Oracle, SQL query

Bioinformatics Tools and Software:

1) **Schrödinger:**

   Maestro, Canvas, Confgen, Desmond, e-Pharmacophore, Glide, Induced Fit, Jaguar, LigPrep, Maestro, Phase, Prime, Protein Preparation Wizard, QikProp, SiteMap, Shape Screening, Water Map, Epik, Bioluminate.

2) **Gromacs, AutoDock, AutoDockVina, FlexX, Pymol, SPDBV, Molinspration, Marvin, VMD, COOT, Avogadro.**
3) **Protein Modelling:**

   I-Tasser, SwissModel, Modeller**.**

Awards and Fellowship:

1) **InSc Research Excellence Award** 2020,
2) **ICMR SRF Award** 2019,
3) Fellowship of **DST-SERB** funded by Department of Science & Technology-Science and Engineering Research Board, Govt. of India, (2016-2019),
4) Fellowship of **NIPER** funded by Ministry of Chemicals and Fertilizers, Govt. of India, during the course of M.S. Pharm, (2014-2016),
5) Qualified **GPAT** 2014,
6) Qualified **NIPER-JEE** 2014.

International Publications:

1. **Lokhande, K.,** Nawani, N., K Venkateswara, S., & Pawar, S. (2020). Biflavonoids from Rhus succedanea as probable natural inhibitors against SARS-CoV-2: a molecular docking and molecular dynamics approach. *Journal of biomolecular structure & dynamics*, 1–13. https://doi.org/10.1080/07391102.2020.1858165.
2. **Lokhande, K. B.,** Apte, G. R., Shrivastava, A., Singh, A., Pal, J. K., K Venkateswara Swamy, & Gupta, R. K. (2020). Sensing the interactions between carbohydrate-binding agents and N-linked glycans of SARS-CoV-2 spike glycoprotein using molecular docking and simulation studies. *Journal of biomolecular structure & dynamics*, 1–19. Advance online publication. https://doi.org/10.1080/07391102.2020.1851303.
3. Gupta, R. K., Apte, G. R., **Lokhande, K. B**., Mishra, S., & Pal, J. K. (2020). Carbohydrate-Binding Agents: Potential of Repurposing for COVID-19 Therapy. *Current protein & peptide science*, 10.2174/1389203721666200918153717. Advance online publication. https://doi.org/10.2174/1389203721666200918153717.
4. **Kiran Bharat Lokhande,** Sangeeta Ballav, Rohit Singh Yadav, K Venkateswara Swamy, Soumya Basu. Probing intermolecular interactions and binding stability of kaempferol, quercetin and resveratrol derivatives with PPAR-γ: docking, molecular dynamics and MM/GBSA approach to reveal potent PPAR- γ agonist against cancer**. (2020),** *Journal of Biomolecular Structure and Dynamics*, 1-11. Doi: 10.1080/07391102.2020.1820380.
5. **Kiran Bharat Lokhande**, Tanushree Banerjee, K Venkateswara Swamy, Manisha Deshpande. An In silico scientific basis for LL-37 as a therapeutic and Vitamin D as preventive for Covid-19. **(2020),** *ChemRxiv (Preprint).* Doi: 10.26434/chemrxiv.12928202.v1.
6. **Kiran Bharat Lokhande**, Sangeeta Ballav, Nachiket Thosar, K Venkateswara Swamy, Soumya Basu. Exploring conformational changes of PPAR-Ɣ complexed with novel kaempferol, quercetin, and resveratrol derivatives to understand binding mode assessment: a small-molecule checkmate to cancer therapy. **(2020),** *Journal of Molecular Modeling*. 26(9):1-12: Doi: 10.1007/s00894-020-04488-0.
7. Afrin Mansuri, **Kiran Lokhande**, Supriya Kore, Swapnil Gaikwad, Neelu Nawani, K Venkateswara Swamy, Manisha Junnarkar, Sarika Pawar. Antioxidant, anti-quorum sensing, biofilm inhibitory activities and chemical composition of Patchouli essential oil: in vitro and in silico approach. **(2020),** *Journal of Biomolecular Structure and Dynamics*, 1-12. Doi: 10.1080/07391102.2020.1810124.
8. **Kiran Bharat Lokhande**, Sayali Doiphode, Renu Vyas, K Venkateswara Swamy. Molecular docking and simulation studies on SARS-CoV-2 Mpro reveals Mitoxantrone, Leucovorin, Birinapant, and Dynasore as potent drugs against COVID-19. **(2020),** *Journal of Biomolecular Structure and Dynamics*, 1-12. Doi: 10.1080/07391102.2020.1805019.
9. Rushikesh Patel, Ajay Kumar, **Kiran Bharat Lokhande**, KV Swamy, Prof Sharma, Nilesh Kumar. Molecular Docking and Simulation Studies Predict Lactyl-CoA as the Substrate for P300 Directed Lactylation. **(2020),** *ChemRxiv (Preprint).* Doi:10.26434/chemrxiv.12770360.v1.
10. Priti Prabhakar Yewale, **Kiran Bharat Lokhande**, Aishwarya Sridhar, Monika Vaishnav, Faisal Ahmad Khan, Abul Mandal, Kakumani Venkateswara Swamy, Jana Jass, Neelu Nawani. Molecular profiling of multidrug-resistant river water isolates:

insights into resistance mechanism and potential inhibitors. **(2020),** *Environmental Science and Pollution Research*, 27(22): 27279-27292. Doi: 10.1007/s11356-019-05738-2.

11. Sagar Rohidas Nagare, **Kiran Bharat Lokhande**, Kakumani Venkateswara Swamy. Molecular docking studies of flavanone and its derivatives on pi3k pathway to search for potential target against cancer. **(2020),** *Journal of Dental Research and Review*, 7(5): S26-S29.
12. Rohit D Gupta, Krish Parekh, Vaishnavi U Warrier, **Kiran Bharat Lokhande,** K Venkateswara Swamy, Rajkumar S Sood, Rajesh Kumar Gupta. Purification and Characterization of Pectins from Abelmoschus esculentus (Okra Pods) and Citrus limetta (Citrus Peels) and in silico Binding Study of Pectin and Pectic Polysaccharides with Galectin-1. **(2020),** *Journal of Dental Research and Review*, 7(5): S41-S48.
13. Sangeeta Ballav, **Kiran Bharat Lokhande**, Ipshita Dabhi, Sonal Inje, Amit Ranjan, K Venkateswara Swamy, Soumya Basu. Designing novel quercetin derivatives as matrix metalloproteinase-9 inhibitors in colon carcinoma: An In vitro and in silico approach. **(2020),** *Journal of Dental Research and Review*, 7(5): S30-S35.
14. Anwesha Deep Dutta, Ajay Kumar, **Kiran Lokhande**, Manmohan Mitruka, Jayanta K Pal, Sachin C Sarode, Nilesh Kumar Sharma. Detection of oncometabolites 1-methylnicotinamide, nicotine imine and N-Methylnicotinium in nails of oral cancer patients and prediction of them as modulators of DNMT1. **(2020),** *medRxiv (Preprint).* Doi: 10.1101/2020.09.20.20198101.
15. Prajkta B Kothawade**, Kiran B Lokhande**, K Venkateswara Swamy, Sohan S Chitlange, Asha B Thomas. Novel nitrogen-containing heterocyclic compounds in GPR109A as an anti-hyperlipidemic: Homology modeling, docking, dynamic simulation studies. **(2020),** *Journal of Research in Pharmacy*, 24(4):451-463. Doi: 10.35333/jrp.2020.193.
16. Ajay Kumar, Jainish Kothari, Sethamma TN Sinchana, **Kiran Lokhande**, KV Swamy, Nilesh Kumar Sharma. Novel antiproliferative tripeptides block AP-1 transcriptional complex by in silico approach. **(2020),** *bioRxiv (Preprint).* Doi:10.1101/2020.05.08.083972.
17. Priti Prabhakar Yewale, **Kiran Bharat Lokhande**, Aishwarya Sridhar, Monika Vaishnav, Faisal Ahmad Khan, Abul Mandal, Kakumani Venkateswara Swamy, Jana Jass, Neelu Nawani. Molecular profiling of multidrug-resistant river water isolates: insights into resistance mechanism and potential inhibitors. **(2020),** *Environ Sci. Pollut. Res.* 1-14. Doi: 10.1007/s11356-019-05738-2.
18. Sneha R Chandani, **Kiran B Lokhande, K Venkateshwara Swamy**, Rabindra K Nanda, Sohan S Chitlange. Data on docking of phytoconstituents of Actinidia deliciosa on dengue viral targets. **(2019),** *Data in Brief,* 24, Article 103996. Doi: 10.1016/j.dib.2019.103996.
19. Sejal P Gandhi, **Kiran B Lokhande**, Venkateswara K Swamy, Rabindra K Nanda, Sohan S Chitlange. Computational data of phytoconstituents from Hibiscus rosa-sinensis on various anti-obesity targets. (2019), *Data in Brief,* 24, Article 103994. Doi: 10.1016/j.dib.2019.103994.
20. **Kiran Bharat Lokhande**, Shuchi Nagar, K Venkateswara Swamy. Molecular interaction studies of Deguelin and its derivatives with Cyclin D1 and Cyclin E in cancer cell signaling pathway: The computational approach. **(2019).** *Scientific Reports,* 9(1), 1-13. Doi: 10.1038/s41598-018-38332-6.

21. Pulakuntla S Reddy, **Kiran Bharat Lokhande**, Shuchi Nagar, Vaddi Damodara Reddy, P Sushma Murthy, K Venkateswara Swamy. Molecular modeling, docking, dynamics and simulation of Gefitinib and its derivatives with EGFR in non-small cell lung cancer. **(2018),** *Curr Comput Aided Drug Des.* 14(3):246-252. Doi: 10.2174/1573409914666180228111433.
22. Gadamsetty Saayi Krushna, Vutharadhi Leela Shivaranjani, Jolapuram Umamaheswari, Cheemanapalli Srinivasulu, Shaik Althaf Hussain, Mohammed Abdul Kareem, Vaddi Damodara Reddy, Daoud Ali, **Kiran Bharat Lokhande**, K Venkateswara Swamy, Lakshmi Devi Kodidhela. In vivo and molecular docking studies using whole extract and phytocompounds of Aegle marmelos fruit protective effects against Isoproterenol-induced Myocardial infarction in rats. **(2017),** *Biomedicine & Pharmacotherapy,* 91:880-889. Doi: 10.1016/j.biopha.2017.04.115.

Abstracts in Conference Proceedings:

1) **Lokhande, Kiran** and Swamy, K. Venkateswara, Molecular Design, Docking and Dynamic Studies of Novel B, C-Ring Truncated Deguelin Derivatives with Cyclin D1 and Cyclin E (January 15, 2020). *Proceedings of International Conference on Drug Discovery (ICDD) 2020*, Available at SSRN: https://ssrn.com/abstract=3527996.
2) K Venkateswara Swamy and **Kiran Bharat Lokhande**. Molecular modeling, docking, dynamics and simulation of deguelin and its derivatives with cyclin D1 and cyclin E in cancer cell signaling pathway. ***J Proteomics Bioinform,*** 10:11(Suppl.), **(2017).** DOI: 10.4172/0974-276X-C1-106.
3) Prachi Bhole, **Kiran Bharat Lokhande**, Shuchi Nagar, K. Venkateswara Swamy. Molecular Docking and Molecular Dynamics Simulation studies of DHFR inhibitors in Plasmodium falciparum. ***Can J Biotech*** **(2017)**, Volume 1, Special Issue, Page 23, DOI: https://doi.org/10.24870/cjb.2017-a11.
4) Rohit Singh Yadav, **Kiran Bharat Lokhande**, Vaddi Damodara Reddy, K. Venkateswara Swamy. Molecular Docking and Molecular Dynamic studies of Phytocompounds with HIF-1α, HIF-2α, and SREBP1c to explore its Inhibitory Effect on Metabolic disorders and in Cancer. ***Can J Biotech*** **(2017)**, Volume 1, Special Issue, Page 25, DOI: https://doi.org/10.24870/cjb.2017-a13.

Seminars/Webinars/Symposium/Conferences/ Workshops:

1) National Symposium on ***"Recent Advances in Modern Biology and Biotechnology 2019",*** organized by Dr. D.Y. Patil Biotechnology and Bioinformatics Institute, Pune, during 14th to 16th March, 2019.
2) ***"Industry-Academia Conclave 2018 (IAC2018)"*** organized by Dr. D.Y. Patil Biotechnology and Bioinformatics Institute, Pune, during 23rd to 24th Feb, 2018.
3) International webinar on ***"An Introduction to Schrödinger's Python API",*** organized by Schrödinger on 11th January, 2018.
4) ***International symposium*** *on* ***"Novel Targets for Cancer Therapy",*** organized by Interdisciplinary science and technology Research Academy (ISTRA), Azam Campus, Pune, held o 5th January 2018.
5) ***"International Conference on Drug Design"*** organized by Schrödinger at Convention Centre, Jawaharlal Nehru University, New Delhi, during 8th to 9th April, 2017.

6) Workshop on ***"Free Energy Perturbations (FEP) for prediction of accurate binding affinity-FEP+, Automated application to build, validate and deploy predictive QSAR models-AutoQSAR, Hydration Thermodynamics-WaterMap, and Efficient mining of protein-ligand complexes based on geometry from biological database-PLDB"*** organized by Schrödinger at Convention Centre, Jawaharlal Nehru University, New Delhi, on 7th April, 2017.
7) ***"Schrödinger's 5th European Life Science Boot camp - a series of interactive webinars"*** These workshops included training on the following tools: Small-Molecule Drug Discovery Suite, Maestro 11, Pharmacophore Modeling with Phase, Polypeptide docking with Glide, and Lead Optimization with WaterMap and FEP+, during 20th March to 24th March, 2017.
8) Webinar on ***"Introduction to Cresset science and software foe academics_2017"*** organized by Cresset on 21st March, 2017.
9) National Symposium on ***"Recent Advances in Modern Biology and Biotechnology 2017",*** organized by Dr. D.Y. Patil Biotechnology and Bioinformatics Institute, Pune, during 16th to 17th March, 2017.
10) International webinar on ***"Lead Optimization with FEP+: Innovation in 2017 and Sneak Peek at 2017"***, Schrödinger's 2017 Spring Seminar Series, Organized by Schrödinger on 7th March, 2017.
11) International webinar on ***"Maestro 11: What's New in 2017"***, Schrödinger's 2017 Spring Seminar Series, organized by Schrödinger on 2nd March, 2017.
12) International webinar on ***"Lead Optimization with FEP+: Innovation in 2017 and Sneak Peek at 2017"***, Schrödinger's 2017 Spring Seminar Series, organized by Schrödinger on 28th February, 2017.

Technical Abstracts/Oral/Poster presentations:

1) **Kiran Bharat Lokhande*** and K. Venkateswara Swamy. ***"Molecular Design, Docking and Dynamic Studies of Novel B, C-Ring Truncated Deguelin Derivatives with Cyclin D1 and Cyclin E".*** International conference on Drug Discovery (ICDD) 2020, organized by Schrödinger Inc, USA in collaboration with BITS Hyderabad, Hyderabad, during Feb 29th- March 2nd, 2020.
2) **Kiran Bharat Lokhande*** and K. Venkateswara Swamy. ***"Structural Basis for Depletion of HIF-1α by Deguelin and its Derivatives in Cancer"*** Organized by NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT 2019) Conference at Taj Land End during Sep 30th – Oct 2nd, 2019.
3) Sayali Doiphode*, **Kiran Bharat Lokhande** and K. Venkateswara Swamy. "***In silico molecular interaction studies of lead compounds with Cytidine/Uridine monophosphate kinase 2 (CMPK2) and Thioredoxin Interacting Protein (TXNIP)".*** Organized by NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT 2019) Conference at Taj Land End during Sep 30th – Oct 2nd, 2019.
4) Khushboo Pandey*, **Kiran Bharat Lokhande**, Arvind Goja and Shuchi Nagar. ***"Selection of novel aromatase inhibitors using molecular docking studies",*** in Accelerating Biology-2019, C-DAC, Pune, organized by Indian Institutes of Science Education and Research (IISER), Pune, during 5th – 7th Feb. **2019.**
5) Sangeeta Ballav*, **Kiran Bharat Lokhande**, Nachiket Thosar, Nishant Lodha, K. Venkateswara Swamy and Soumya Basu. ***"In silico studies of Kaempferol, Quercetin, Resveratrol and their derivatives with PPAR-γ as a therapeutic target in cancer,"*** in

XLII All India Cell Biology Conference and 2nd international conference- The Cell in Action: Trends in Cell and Molecular Biology. Organized by All India Cell Biology Society, at Department of Biological Sciences, BITS Pilani, K K Birla Goa campus. 21st – 23rd Dec. **2018.**

6) **Kiran Bharat Lokhande***, Sangeeta Ballav, Rohit Singh Yadav, Amit Ranjan, K. Venkateswara Swamy and Soumya Basu. ***"Studies of Kaempferol, Quercetin, Resveratrol and their derivatives with PPAR-gamma as a therapeutic target in cancer: An in silico Approach"*** in Indo-Australia Symposium on "Epithelial-Mesenchymal Transition" held on 24th October **2018** at National Centre for Cell Science, Pune, India.
7) **Kiran Bharat Lokhande*** and K. Venkateswara Swamy. ***"Structural basis for pAkt, TNFR1, TRADD receptors and anti-cancer activity of Deguelin and its derivatives",*** organized by NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT) Conference, SciGenom Research Foundation (SGRF) at Fairmont Jaipur, India. 30th Oct. – 2nd Nov. 2018.
8) Mayuri Hendricks*, **Kiran Bharat Lokhande** and K. Venkateswara Swamy. ***"Integrated Homology Modelling and In-Silico Analysis of CPA3",*** organized by NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT) Conference, SciGenom Research Foundation (SGRF) at Fairmont Jaipur, India. 30th Oct. – 2nd Nov. **2018.**
9) Diksha Patil*, **Kiran Bharat Lokhande** and K. Venkateswara Swamy. ***"In silico studies on the inhibitory mechanism of JQ1 and its derivatives in Anaplastic Thyroid Cancer against DNA replication licensing factor (MCM5)",*** organized by NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT) Conference, SciGenom Research Foundation (SGRF) at Fairmont Jaipur, India. 30th Oct. – 2nd Nov. **2018.**
10) Alquama Lokhandwala*, **Kiran Bharat Lokhande** and K. Venkateswara Swamy. ***"In silico studies on the inhibitory mechanism of Carmofur and its derivatives in pediatric Gliobastoma against Acid Ceramidase (ASAH1)"***, organized by NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT) Conference, SciGenom Research Foundation (SGRF) at Fairmont Jaipur, India. 30th Oct. – 2nd Nov. **2018**.
11) Ajinkya Sunil Mehere*, Amresh Kumar Yadav, **Kiran Bharat Lokhande** and K. Venkateswara Swamy. ***"Molecular Modeling and Docking Studies of Aromatase Inhibitors with Aromatase for ERP Breast Cancer"*** in 86th Conference of Society of Biological Chemists (SBC) - Emerging Discoveries in Health and Agricultural Sciences organized by School of Life Sciences, Jawaharlal Nehru University, New Delhi, during 16th – 19th Nov., **2017.**
12) K. Venkateswara Swamy* and **Kiran Bharat Lokhande.** ***"Molecular modeling, docking, dynamics and simulation of Deguelin and its derivatives with cyclin D1 and cyclin E in cancer cell signaling pathway",*** in 9th International Conference and Expo on Proteomics and Molecular Medicine & 9th International Conference on Bioinformatics, at France, Paris. 13th – 15th Nov., **2017.**
13) Rohit Singh Yadav*, **Kiran Bharat Lokhande**, Vaddi Damodara Reddy, K. Venkateswara Swamy. ***"Molecular docking and Molecular Dynamics studies of phytocompounds with HIF-1α, HIF-2α and Srebp1c to explore its inhibitory effect on metabolic disorder and in cancer",*** in 2017 NextGen Genomics, Biology,

Bioinformatics and Technologies (NGBT) organized by SGRF, at Bhubaneswar, Odisha, India. 1st - 4th Oct, **2017**.

14) Prachi Bhole*, **Kiran Bharat Lokhande**, Shuchi Nagar and K. Venkateswara Swamy. *"**Molecular Docking and Molecular Dynamics Simulation studies of DHFR inhibitors in Plasmodium falciparum"***, in 2017 NextGen Genomics, Biology, Bioinformatics and Technologies (NGBT) organized by SGRF, at Bhubaneswar, Odisha, India. 1st - 4th Oct, **2017**.

15) **Kiran Bharat Lokhande*** and K. Venkateswara Swamy **"*Molecular Modeling, Docking, Dynamics and Simulation of Deguelin and Its Derivatives with Cyclin D1 and Cyclin E In Cancer Cell Signaling Pathway"*** in International Conference on Drug Design, at Convention Centre, Jawaharlal Nehru University, New Delhi, on 8th April, **2017**.