Mr. KIRAN BHARAT LOKHANDE

Designation   :   **Senior Research Fellow**

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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 Investigato**r: **Dr. K. Venkateswara. Swamy**, Associate Professor, Bioinformatics Research Laboratory

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

International Publications:

1. 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. **(2019),** *Environ Sci. Pollut. Res.* 1-14. Doi: 10.1007/s11356-019-05738-2.

2. 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.

3. 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.

4. **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.

5. 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.

6. 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) 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.

2) 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.

3) 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) 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.**

2) 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.**

3) **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.

4) **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.

5) 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.**

6) 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.**

7) 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**.

8) 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.**

9) 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.**

10) 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**.

11) 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**.

12) **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**.