

## Mr. KIRAN BHARAT LOKHANDE

**Designation** : Junior Research Fellow

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**Phone Number** : 020-67919444 Extn. -9449

**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:

**Junior Research Fellow (JRF)** | Bioinformatics Research Laboratory  
Dr. D.Y. Patil Biotechnology and Bioinformatics Institute (Oct. 2016 – Present).

**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. V. 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) Qualified **GPAT** 2014
- 2) Qualified **NIPER-JEE** 2014
- 3) Fellowship of **NIPER** funded by Ministry of Chemicals and Fertilizers, Govt. of India, during the course of M.S. Pharm, (2014-2016).

## International Publications:

- 1) 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 (2017). In vivo and molecular docking studies using whole extract and phytochemicals of *Aegle marmelos* fruit protective effects against Isoproterenol-induced Myocardial infarction in rats. *Biomedicine & Pharmacotherapy* 91:880–889. PMID: 28511341, DOI: 10.1016/j.biopha.2017.04.115. (Impact factor: 2.326).

## Seminars/Webinars/Symposium/Conferences/ Workshops:

- 1) “**International Conference on Drug Design**” organized by Schrödinger at Convention Centre, Jawaharlal Nehru University, New Delhi, during 8<sup>th</sup> to 9<sup>th</sup> April, 2017.

- 2) 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 7<sup>th</sup> April, 2017.
- 3) **“Schrödinger’s 5<sup>th</sup> 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 20<sup>th</sup> March to 24<sup>th</sup> March, 2017.
- 4) Webinar on **“Introduction to Cresset science and software for academics\_2017”** organized by Cresset on 21<sup>st</sup> March, 2017.
- 5) National Symposium on **“Recent Advances in Modern Biology and Biotechnology 2017”**, organized by Dr. D.Y. Patil Biotechnology and Bioinformatics Institute, Pune, during 16<sup>th</sup> to 17<sup>th</sup> March, 2017.
- 6) 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 7<sup>th</sup> March, 2017.
- 7) International webinar on **“Maestro 11: What’s New in 2017”**, Schrödinger’s 2017 Spring Seminar Series, organized by Schrödinger on 2<sup>nd</sup> March, 2017.
- 8) 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 28<sup>th</sup> February, 2017.

### **Technical Abstracts/Oral/Poster presentations in India:**

- 1) Poster presentation on **“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 8<sup>th</sup> April, 2017.