Dr. D.Y. Patil Vidyapeeth's
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Mr. KIRAN BHARAT LOKHANDE

Designation : Junior Research Fellow

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

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 phytocompounds 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).**

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) International webinar on **"An Introduction to Schrödinger's Python API",** organized by Schrödinger on 11th January, 2018.
2) **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.
3) **"International Conference on Drug Design"** organized by Schrödinger at Convention Centre, Jawaharlal Nehru University, New Delhi, during 8th to 9th April, 2017.
4) 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.
5) **"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.
6) Webinar on **"Introduction to Cresset science and software foe academics_2017"** organized by Cresset on 21st March, 2017.
7) 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.
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 7th March, 2017.
9) International webinar on **"Maestro 11: What's New in 2017"**, Schrödinger's 2017 Spring Seminar Series, organized by Schrödinger on 2nd 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 28th February, 2017.

Technical Abstracts/Oral/Poster presentations:

1) *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.

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",** in 9th International Conference and Expo on Proteomics and Molecular Medicine & 9th International Conference on Bioinformatics, at France, Paris. 13th – 15th Nov., 2017.
3) *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.
4) *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.
5) ***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.