PERSONAL INFORMATION

BALASUBRAMANIYAN SAKTHIVEL

Native address (Home): Thanjavur, Tamilnadu, INDIA

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https://www.linkedin.com/in/bala-s-ph-d-a6b68470/

Sex Male | Date of birth 15/03 /1988 | Nationality Indian

WORK EXPERIENCE

May 2024 - Present

Postdoctoral Researcher
Institute for Chemical Reaction Design and Discovery (ICReDD)
Hokkaido University, Sapporo - Japan
Analysis and modeling of experimental data in collaboration with robotic synthesis platform.

December 2021- November 2023

Senior Research Scientist
Computational Chemistry-CADD
Anticancer Bioscience-Chengdu, China
Target identification, Drug Design, Chemical hit and lead generation, Lead optimization
Organic Synthesis (Discovery of small molecule cancer drugs)

May 2020- November 2021

Research Associate
Computational Chemistry-CADD
D3 Drug Lab Pvt. Ltd. Chennai, India.
Drug Design, Virtual Screening, Chemical hit and lead generation, Organic Synthesis.

EDUCATION

Jully 2014- March 2021

Ph.D.-Doctor of Philosophy
Drug Discovery and Development Research Group
Department of Pharmaceutical Technology, Anna University, Trichy, India

September 2011- November 2012

M.Phil. Master of Philosophy
The Gandhigram Rural Institute- Dindigul. India

August 2009- June 2011

M.Sc.-Master of Science in Chemistry, First Class
Periyar E.V.R. College, Bharathidasan University -Trichy, India

June 2006- July 2009

B.Sc.- Bachelor of Science in Chemistry, First Class
Govt. Arts College, Bharathidasan University -Trichy, India

RESEARCH INTEREST

- De novo - ligand- and fragment-based drug discovery
- Finding new molecules to combat emerging diseases
- Predict the biological activity of the new molecules
- Identification of Hit molecules, Hit to Lead generation/optimization
- Organic Synthesis and Characterization Techniques

Title of Ph.D. thesis work

In silico design, synthesis and biological evaluation of novel fluoroquinolone analogs with improved potency against fluoroquinolone-resistant Escherichia coli for the treatment of urinary tract infections.

RESEARCH EXPERTISE

Industrial Research Experience
Design new bioactive molecules - protein-ligand interactions - identify the target protein for new scaffold molecules-Structure/Ligand-based pharmacophore analysis - Pharmacokinetic/metabolism site prediction - protein homology modeling - Hit to Lead generation/optimization -synthesis of small molecules.

Doctoral Research (Anna University, India)

Discovery of new fluoroquinolone analogs with improved potency against fluoroquinolone-resistant Escherichia coli. Mainly, new inhibitors for mutant DNA gyrase target enzymes were discovered using structure and ligand-based drug design approaches.

- Homology modeling of the target protein
- Structure and Ligand-based drug design
- Virtual screening of designed molecules using molecular docking, MD Simulation pharmacophore, QSAR, and ADMET analysis
- Synthesis of the virtually screened molecules

PROFESSIONAL SKILLS

- Homology modeling
- De Novo & ligand-based drug design
- Molecular Docking
- MD Simulation and free energy calculations
- Pharmacophore & QSAR modeling
- Drug Target Identification
- ADMET Prediction
- Virtual screening of drug molecules
- Hit to Lead generation/optimization
- Multi-step organic synthesis

Mother Tonge Tamil

Other Languages (s) English (Advanced Level)

Communication Skill Excellent presentation skills demonstrated in various meetings and national, and international

Organizing skills Involved as an organizing member in conducting several national and international conferences

Software skills Computer-Aided Drug Design Software

- BIOVIA Discovery Studio
- Maestro - Schrodinger
- Forecaster

Programming Skills Python

PUBLICATIONS

13. Venkatesh, G., Vennila, P., & **Balasubramaniyan, S.** (2024). Solvent effects, chemical reactivity, docking and antimicrobial activity of silver and gold nanocages glimepiride: Experimental and theoretical calculations. *Chemical Physics Impact*, (**IF: 2.2**), *8*, 100498. Link: https://www.sciencedirect.com/science/article/pii/S2667022424000422

12. Li, J., Zhang, T., Shi, Q., Lv, G., Zhou, X., Choudhry, N., Kalashova, J., Yang, C., Li, H., Long, Y. and **Balasubramaniyan.S**, 2023. Orally Bioavailable 4-Phenoxy-quinoline Compound as a Potent Aurora Kinase B Relocation Blocker for Cancer Treatment. *ACS Pharmacology & Translational Science* (**IF: 1.67**), *6*(8), pp.1155-1163. Link: https://pubs.acs.org/doi/abs/10.1021/acsptsci.3c00054

11. Nagendran, Saraswathy, **Sakthivel Balasubramaniyan**, and Navabshan Irfan. "Virtually screened novel sulfathiazole derivatives as a potential drug candidate for methicillin-resistant Staphylococcus aureus and multidrug-resistant tuberculosis." *Journal of Biomolecular Structure and Dynamics* (**IF: 5.23**) 41, no. 11 (2023): 5086-5095. Link: https://www.tandfonline.com/doi/abs/10.1080/07391102.2022.2079002

10. Kotakonda, Muddukrishnaiah, Makesh Marappan, Prabaharan Dharmar, **Balasubramaniyan Sakthivel**, and Prasad Sunnapu. "Isolation and Identification of Bioactive Compounds with Antimicrobial Activity from Marine Facultative Anaerobe, Bacillus subtilis." *Current Pharmaceutical Biotechnology* (**IF: 2.89**) 24, no. 5 (2023): 698-707.
Link: https://pubmed.ncbi.nlm.nih.gov/35927910/

9. Kumar, Praveen, Santhosha Sangapurada Mahantheshappa, **Sakthivel Balasubramaniyan**, Nayak Devappa Satyanarayan, and Rajeshwara Achur. "Quinoline analogue as a potential inhibitor of SARS-CoV-2 main protease: ADMET prediction, molecular docking and dynamics simulation analysis." *European Journal of Chemistry* (**IF: 0.6**)14, no. 1 (2023): 30-38.
Link: https://www.eurjchem.com/index.php/eurjchem/article/view/2350

8. Irfan, Navabshan, **Sakthivel Balasubramaniyan***, Davoodbasha Mubarak Ali, and Ayarivan Puratchikody. "Bioisosteric replacements of tyrosine kinases inhibitors to make potent and safe chemotherapy against malignant cells." *Journal of Biomolecular Structure and Dynamics* (**IF: 5.23**) (2022): 1-11.
Link: https://www.tandfonline.com/doi/abs/10.1080/07391102.2022.2146751

7. Santhaseelan, Henciya, Vengateshwaran Thasu Dinakaran, **Balasubramaniyan Sakthivel**, Maharaja Somasundaram,"Bioactive Efficacy of Novel Carboxylic Acid from Halophilic Pseudomonas aeruginosa against Methicillin-Resistant Staphylococcus aureus." *Metabolites* (**IF:5.58**)12, no. 11 (2022): 1094.
Link: https://www.mdpi.com/2218-1989/12/11/1094

6. Sugumaran, Abimanyu, Rajesh Pandiyan, Palanivel Kandasamy, Mariya Gover Antoniraj, Irfan Navabshan, **Balasubramaniyan Sakthivel**, Selvakumar Dharmaraj, Santhosh Kumar Chinnaiyan, Veeramuthu Ashokkumar, and Chawalit Ngamcharussrivichai. "Marine biome-derived secondary metabolites, a class of promising antineoplastic agents: A systematic review on their classification, mechanism of action and future perspectives." *Science of The Total Environment* 836 (**IF:10.75**) (2022): 155445.
Link: https://www.sciencedirect.com/science/article/abs/pii/S0048969722025396

5. Muthukumar, C., **S. Balasubramaniyan**, Deviram Garlapati, M. Durga Bharathi, B. Charan Kumar, R. A. James, K. Ramu, and M. V. Ramanamurthy. "Impact of untreated sewage and thermal effluent discharges on the air-sea CO2 fluxes in a highly urbanized tropical coastal region." *Marine Pollution Bulletin* (**IF:7.00**)175 (2022): 113166. Link: https://www.sciencedirect.com/science/article/abs/pii/S0025326X21012005

4. Navabshan, Irfan, **Balasubramaniyan Sakthivel**, Rajesh Pandiyan, Mariya Gover Antoniraj, Selvakumar Dharmaraj, Veeramuthu Ashokkumar, Kuan Shiong Khoo, Kit Wayne Chew, Abimanyu Sugumaran, and Pau Loke Show. "Computational lock and key and dynamic trajectory analysis of natural biophors against COVID-19 spike protein to identify effective lead molecules." *Molecular biotechnology* (**IF2.86**) 63, no. 10 (2021): 898-908.
Link: https://link.springer.com/article/10.1007/s12033-021-00358-z

3. **Balasubramaniyan Sakthivel**, Navabshan Irfan, Chinnaiyan Senthilkumar, Appavoo Umamaheswari, and Ayarivan Puratchikody. "The synthesis and biological evaluation of virtually designed fluoroquinolone analogs against fluoroquinolone-resistant Escherichia coli intended for UTI treatment." *New Journal of Chemistry* **(IF:3.92)** 44, no. 31 (2020): 13308-13318.
Link: https://pubs.rsc.org/en/content/articlelanding/2020/nj/d0nj00657b/unauth

2. Puratchikody, Ayarivan, Navabshan Irfan, and **Sakthivel Balasubramaniyan**. "Conceptual design of hybrid PCSK9 lead inhibitors against coronary artery disease." *Biocatalysis and Agricultural Biotechnology* (**IF:4.00**)17 (2019): 427-440.
Link: https://www.sciencedirect.com/science/article/abs/pii/S1878818118306595

1. **Balasubramaniyan Sakthivel**, Navabshan Irfan, Appavoo Umamaheswari, and Ayarivan Puratchikody. "Design and virtual screening of novel fluoroquinolone analogs as effective mutant DNA GyrA inhibitors against urinary tract infection-causing fluoroquinolone resistant Escherichia coli." *RSC advances* (**IF:4.03**) 8, no. 42 (2018): 23629-23647.
Link: https://pubs.rsc.org/en/content/articlehtml/2017/sc/c8ra01854e

Book Chapters

1. Ramalakshmi, N., S. Arunkumar, and **S. Balasubramaniyan**. "QSAR and Lead Optimization. InComputer Applications in Drug Discovery and Development 2019 (pp. 80-100).

2. Umamaheswari, A., A. Puratchikody, and **Sakthivel Balasubramaniyan**. "Target Identification of HDAC8 Isoform for the Treatment of Cancer." In *Computer Applications in Drug Discovery and Development*, pp. 140-172. IGI Global, 2019.
Link:https://www.igi-global.com/chapter/target-identification-of-hdac8-isoform-for-the-treatment-of-cancer/217072

Reviewer

Royal Society of Chemistry, Springer and Taylor &Francis journals

References

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