Dr. Syed Jawad Ali Shah
Assistant Professor Pharmaceutical Chemistry,
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Education

- **PhD** (2022): Medicinal Chemistry and Biology, School of Pharmacy, Lanzhou University, China.
  Thesis title: Molecular Dynamics Simulation Study of the Effect of Acetylation on Misfolding and Aggregation of Tau Protein
- **M.Phil.** (2015): COMSATS University Islamabad, Abbottabad Campus.
  Thesis title: Identification of Novel Derivatives as Potent Inhibitors of Cholinesterases, their Enzyme Kinetics and Molecular Docking Studies

Professional Experience

- **Assistant Professor Pharmaceutical Chemistry,** Department of Pharmacy, PAF-IAST **(Dec 2023 to date).**
- **Assistant Professor/Section Head Pharmaceutical Chemistry,** Department of Pharmacy, The University of Lahore. **(Nov 2022 to Nov 2023).**
- **Research Associate,** Center for Advanced Drug Research, CUI, Abbottabad Campus **(Sep 2015 to Oct 2022).**
- **Visiting Junior Researcher,** Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences, University of Heidelberg (**July 2016 to Sep 2016**)
- **Research Trainee,** BIT – LIMES Institute of University of Bonn, Germany – DAAD funded **(June 2015 to August 2015)**
- **Research Trainee,** Department of Pharmacy, University of Bonn, Germany – DAAD funded **(June 2014 to August 2014)**

Award

- Awarded access to scientific computing under "Red Española de Supercomputación (RES)", Spain.
- Awarded research visit grant by HPC-Europa3 to carry out research project in Barcelona Super Computing (BSC) Center.
- Awarded Chinese Government Scholarship by Chinese Scholarship Council, China for PhD studies.

Research Publications

23 International Publications in ISI indexed journals, impact factor of greater than **96**, citations **285**, *h*-index **11.** Organized and participated in more than **15** national and international conferences as a participant and keynote speakers.

Selected Publications

1. **Shah, S.J.A.,** Zhang, Q., Guo, J., Liu, H., Liu, H. and Villà-Freixa, J., 2023. Identification of Aggregation Mechanism of Acetylated PHF6* and PHF6 Tau Peptides Based on Molecular Dynamics Simulations and Markov State Modeling. ACS Chemical Neuroscience, 14(21), pp.3959-3971. (Impact factor 5.9)
2. **Shah, S.J.A.,** Zhong, H., Zhang, Q. and Liu, H., 2022. Deciphering the Effect of Lysine Acetylation on the Misfolding and Aggregation of Human Tau Fragment 171IPAKTPPAPK180 Using Molecular Dynamic Simulation and the Markov State Model. International Journal of Molecular Sciences, 23(5), p.2399. (Impact factor 6.2)
3. Mahmood, A., **Shah, S.J.A**. and Iqbal, J., 2022. Design and synthesis of adamantane-1-carbonyl thiourea derivatives as potent and selective inhibitors of h-P2X4 and h-P2X7 receptors: An Emerging therapeutic tool for treatment of inflammation and neurological disorders. European Journal of Medicinal Chemistry, 231, p.114162. (Impact factor 7.08)
4. **Shah, S.J.A.,** Iqbal, J. and 2018. Molecular dynamic simulations reveal structural insights into substrate and inhibitor binding modes and functionality of Ecto-Nucleoside Triphosphate Diphosphohydrolases. Scientific Reports, 8(1), p.2581.
5. Khan, I., **Shah, S.J.A.,** Ejaz, S.A., Ibrar, A., Hameed, S., Lecka, J., Millán, J.L., Sévigny, J. and Iqbal, J., 2015. Investigation of quinoline-4-carboxylic acid as a highly potent scaffold for the development of alkaline phosphatase inhibitors: synthesis, SAR analysis and molecular modelling studies. RSC advances, 5(79), pp.64404-64413. (Impact factor 4.036)