Dr. Sumra Wajid Abbasi
Assistant Professor
Biological Sciences

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Specialization:
Computer Aided Drug Designing

Education:
PhD Bioinformatics (2012 - 2016), National Center for Bioinformatics, Quaid-i-Azam University Islamabad, Pakistan.
MS Bioinformatics (2009 - 2012), International Islamic University Islamabad, Pakistan.
BS (Hons) Bioinformatics (2005 - 2009), International Islamic University Islamabad, Pakistan.

Experience:

Assistant Professor (2018 – To date), National University of Medical Sciences, Rawalpindi, Pakistan.

Assistant Professor (2017 – 2018), National Center for Bioinformatics, Quaid-i-Azam University, Islamabad, Pakistan.

Research Interests:
Homology Modelling, Ab Initio Protein Structure Prediction, Virtual Screening, Compound Synthesis, Reverse Vaccinology, Protein-ligand Docking, Protein-Protein Docking, Molecular Dynamic Simulations of proteins, Hybrid Quantum Mechanical / Molecular Mechanical (QM/MM).

Publications:

1. **Targeting isoprenoid biosynthesis pathway in Staphylococcus lugdunensis: Comparative docking and simulation studies of conventional and allosteric sites.**
   Nousheen Parvaiz, **Sumra Wajid Abbasi**, Reaz Uddin, Syed Sikander Azam (2018). Journal of Molecular Liquids, 269, 426-440. doi: 10.1016/j.molliq.2018.08.072.

2. **Identification of natural inhibitors against Acinetobacter baumannii D-alanine-Dalanine ligase enzyme: A multi-spectrum in silico approach.**
   Sajjad Ahmad, Saad Raza, **Sumra Wajid Abbasi**, Syed Sikander Azam (2018). Journal of Molecular Liquids, 262: 460–475. doi.org/10.1016/j.molliq.2018.04.124.
3. **Phylogenetic analysis, structure modeling and docking study of HCV NS3 protease for the identification of potent inhibitors.**
   Asad Zia, **Sumra Wajid Abbasi,** Shabeer Ahmad, Muhammad Zia, and Abida Raza (2018). Infection, Genetics and Evolution 59: 51-62.
4. **Interaction mechanisms of a melatonergic inhibitor in the melatonin synthesis pathway.**
   Sumra Wajid Abbasi, Saad Raza, Syed Sikander Azam, Klaus R. Liedl, Julian E. Fuchs. (2016). Journal of Molecular Liquids, 221: 507–517. DOI:10.1016/j.molliq.2016.06.034.

5. **A perspective on structural and computational work on collagen.**
   Carmen Domene, Christian Jorgensena and **Sumra Wajid Abbasi**. (2016). Physical Chemistry Chemical Physics, 18: 24802-24811. DOI: 10.1039/c6cp03403a.

6. **Structural Characterization of Alphamethylacyl-CoA Racemase: Comparative Structural Modeling, Molecular Docking and Dynamic Simulations Studies.**
   Sumra Wajid Abbasi and Azam SS. (2015). Current Cancer Drug Targets, 15(9):822-35.

7. **Structural and dynamical aspects of Streptococcus gordonii FabH through molecular docking and MD simulations.**
   Shamim A, **Sumra Wajid Abbasi**, Azam SS. (2015). Journal of Molecular Graphics and Modelling, 60: 180–196. DOI: 10.1016/j.jmgm.2015.05.013.

8. **Investigation of Novel Chemical Inhibitors of Human Lysosomal Acid Lipase: Virtual Screening and Moleculer Docking Studies**.
   Azam SS, **Sumra Wajid Abbasi**, Tahir S. (2014). Combinatorial Chemistry& High Throughput Screening, 17:473-482.

9. **Comparative modeling and molecular docking studies of D-Alanine:D-alanine ligase: a target of antibacterial drugs.**
   Azam, S.S., **Sumra Wajid Abbasi**, Akhtar, A.S. et al. (2014). Medicinal Chemistry Research, 23 (9): 4108-4137. DOI:10.1007/s00044- 014-0970-8.

10. **Molecular docking studies for the identification of novel melatoninergic inhibitors for acetylserotonin-O-methyltransferase using different docking routines.**
    Azam and **Sumra Wajid Abbasi**. (2013). Theoretical Biology and Medical Modelling, 10:63. DOI:10.1186/1742-4682-10-63.

11. **Structure modeling and docking study of HCV NS5B-3a RNA polymerase for the identification of potent inhibitors.**
    Azam S.S., **Sumra Wajid Abbasi,** Batool M. (2013). Medicinal Chemistry Research, 23 (2): 618-627. DOI:10.1007/s00044-013-0666-5.

12. **In silicopharmacophore model generation for the identification of novel butyrylcholinesterase inhibitors against Alzheimer's disease.**
    Sumra Wajid Abbasi, Kulsoom, S. &Riaz, N. (2012). Medicinal Chemistry Research, 21: 2716- 2722.DOI:10.1007/s00044-011-9795-x.