

Dr. Arslan Sehgal

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Google Scholar:

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Profile Summary

Computational biologist specializing in computer-aided drug design (CADD) and structural bioinformatics, with expertise in molecular docking, molecular dynamics simulations, and virtual screening for therapeutic discovery. My research focuses on identifying novel drug candidates and vaccine targets for complex diseases, including cancer, neurodegenerative disorders, and infectious diseases. I have authored 68+ peer-reviewed publications (h-index =26), reflecting strong contributions to computational pharmacology and translational bioinformatics. My PhD from the University of Chinese Academy of Sciences focused on structure-based inhibition of mitophagy pathways (LC3–FUNDC1 interaction) and the verification of the screened compounds through wet-lab experiments. I also have experience in NGS-based genomic and metagenomic data analysis, including 16S rRNA microbiome profiling (OTU/ASV analysis), as well as clinical exome and whole genome sequencing (WGS) for variant identification (SNPs, CNVs) and annotation.

Research Interests

- Computer-aided drug design (CADD) for cancer, neurological, and mitochondrial disorders
- Development of bioassays and computational pipelines for therapeutic screening
- Subtractive genomics, comparative genomics, and reverse vaccinology for drug and vaccine discovery
- Immunoinformatics and epitope-based vaccine/drug design
- Next-Generation Sequencing (NGS)-based genomic and metagenomic data analysis
- Gut microbiome profiling using 16S rRNA sequencing, including OTU/ASV-based diversity and community structure analysis
- Clinical exome sequencing for identification and annotation
- Whole genome sequencing (WGS) analysis for detection of SNPs and CNVs

Education

PhD Cell Biology (Bioinformatics)

University of Chinese Academy of Sciences, Beijing China (2015-2019)

Thesis: *Screening of novel compounds that target the interaction of LC3 and FUNDC1 for inhibition of Auto(mito)phagy*

Supervisor: Professor Dr. Quan Chen, Professor Dr. TieshanTang

MS Bioinformatics

International Islamic University Islamabad, Islamabad, Pakistan (2011-2013)

BS Bioinformatics

Government College University Faisalabad, Faisalabad, Pakistan (2006-2010)

Professional Experience

Assistant Professor (BPS-19)

Cholistan University of Veterinary and Animal Sciences (03 April, 2024-Present)

Lecturer (BPS-18)

The Islamia University of Bahawalpur (11 April, 2022-02 April, 2024)

Assistant Professor (IPEP and Visiting)

University of Okara (Aug. 2020- April 2022)

Assistant Professor (Visiting)

Government College University Faisalabad (Aug 2019- Aug 2020)

Lecturer (OG II)

COMSATS University Islamabad, Sahiwal Campus (Feb. 2015- Sep. 2020)

Research Projects (Grants)

PI – Computational Drug Design for Mitophagy (HEC Funded)

Identification of novel compounds targeting LC3–FUNDC1

Research Metrics

Total Publications: 68

Cumulative Impact Factor: >215

Citations: >2250

h-index: 26

i10-index: 38

Selected Publications

Corresponding Author

- ***In silico* Identification and Computational Screening of Potential AFP Inhibitors Against Liver Cancer.** *Medicinal Chemistry* 2025 21 (6), 554-565 (IF: 2.6)
- ***In silico* identification and virtual screening to discover potent therapeutic phytochemicals against CMT2A.** *Journal of the Indian Chemical Society* 2024 (IF: 3.2)
- **Immunoinformatics and Molecular Docking Studies Predicted Potential Multiepitope-Based Peptide Vaccine and Novel Compounds against Novel SARS-CoV-2 through Virtual Screening.** *BioMed Research International*, 2021, (IF: 3.411)
- **Determine the potential Epitope based Peptide Vaccine against novel SARS-CoV-2 targeting structural proteins using immunoinformatics approaches.** *Frontiers in Molecular Biosciences*, 2020, 7, 227 (IF: 5.246)
- **Ligand-Based Pharmacophore Modeling and Virtual Screening to Discover Novel CYP1A1 Inhibitors.** *Current Topics in Medicinal Chemistry*, 2019, 19 (30), 2782-2794. (IF: 3.295)
- **Pharmacoinformatics and molecular docking reveal potential drug candidates against Schizophrenia to target TAAR6.** *Journal of Cellular Physiology*, 2019, 234 (8), 13263-13276. (IF: 6.384)

- **Immunoinformatics and molecular docking studies reveal potential Epitope based Peptide Vaccine against DENV-NS3 Protein.** *Journal of Theoretical Biology*, 2018, 459, 162-170. (IF: 2.691)
- **Pharmacoinformatics, Adaptive Evolution, and Elucidation of Six Novel Compounds for Schizophrenia Treatment by Targeting DAOA (G72) Isoforms.** *BioMed Research International*, 2017, Article ID 5925714, doi:10.1155/2017/5925714. (IF: 3.411)

Principal Author

- **Adaptive Evolution and elucidating the potential inhibitor against Schizophrenia to target DAOA (G72) Isoforms.** *Drug Design Development and Therapy* 2015, 9, 3471 (IF: 4.162)
- **Pharmacoinformatics elucidation of potential drug targets against migraine to target ion channel protein KCNK18.** *Drug Design Development and Therapy* 2014 8, 571-581. (IF: 4.162)

Co-Author

- **The long noncoding RNA SNHG12 defines KEAP1 stability and ferroptosis susceptibility by targeting E3 ligase TRIM25** *Journal of Biological Chemistry* 2025, 110689 (IF: 3.4)
- **The multifaceted regulation of mitophagy by endogenous metabolites.** *Autophagy*, 2022,18 (6) 1216-1239 (IF: 16.016)
- **Defective mitochondrial ISCs biogenesis switches on IRP1 to fine tune selective mitophagy.** *Redox Biology*, 2020, 101661 (IF: 11.799)
- **STING directly activates autophagy to tune the innate immune response.** *Cell Death and Differentiation* 2019, 26 (9), 1735-1749 (IF: 15.828)
- **Mitochondrial E3 ligase MARCH5 regulates FUNDC1 to fine-tune hypoxic mitophagy.** *EMBO reports*, 2017, 18(3), 495-509 p.e201643309. (IF: 8.807)

Technical Skills

Wet Lab

- DNA/RNA extraction
- PCR, qPCR
- Gel electrophoresis
- ELISA, Western blotting

Dry Lab (Bioinformatics)

- QIIME2 (microbiome analysis)
- Molecular docking (AutoDock, PyRx, MOE)
- Molecular dynamics simulation (Desmond)
- R (phyloseq, ggplot2)
- BLAST, ClustalW, MEGA

Achievements and Awards

- Excellent International Student Award – UCAS (2018)
- Multiple Research Productivity Awards (CUI (2015, 2016, 2017))
- Best Poster Awards (2014, 2022, 2023)

Books

- **Quick Guideline for Computational Drug Design** (Bentham Science, 2018)
- **Quick Guideline for Computational Drug Design** (Bentham Science, Revised Edition 2021)

International Exposure

- PhD – China (UCAS, CAS collaboration)
- Conferences in China and Singapore

Teaching & Supervision

- 200+ credit hours taught
- Supervised BS, MS, and PhD research students