Maria Batool

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Professional Summary

A goal-driven research scientist with vast exposure in drug discovery and have the perseverance to meet milestones. I enjoy leading multi-disciplinary project teams from target identification and validation through candidate selection. Primary skills include structure-based drug design, understanding of protein folding mechanisms, and molecular dynamics. Analytical experience includes solving protein structure issues, virtual compound design, screening, modification, and leads optimization.

Research Interests

Interested in machine learning-based small molecules and peptides-based drug designing as well as the use of computational techniques to understand the protein folding and dynamic behavior of molecules.

Professional Experiences

- **Planned Career Break** Nov, 2021 - Present
  - I took a planned brief career break (one and a half year) off to care for my child, and now I'm very excited about returning to work!
- **Postdoctoral Research Associate** Feb, 2021 - Oct, 2021
  Ajou University *Suwon, South Korea*
  - Implementation and optimization of computational modeling methods for enhanced identification of peptides and small molecules.
  - Computational analysis of multiomics data from human gut microbiome.
  - Network analysis of protein-protein interactions.
- **Research Scientist** Sept, 2020 - Jan, 2021
  S&K Therapeutics *Suwon, South Korea*
  - Managing cross-functional project teams in the autoimmune and anti-viral therapeutic areas to discover candidate compounds.
  - Visualization of macro molecular complexes at atomic resolution for knowledge-based design.
  - Molecular dynamics and analysis of biomolecular membranes.
  - Protein modeling, data mining, and virtual screening techniques to identify leads.
  - Optimization and modification of existing chemical series to design novel chemotypes.
- **Research Fellow** 2015 - 2020
  Innate Immunity, Cell Signaling and Computational Biology Lab, Ajou University *Suwon, South Korea*
  - Worked on the development of therapeutics to tackle autoimmune disorders and infectious diseases. My major role was to design small molecules or peptide-based drugs using computational techniques. In addition, actively studied dynamic behavior of proteins and receptors for better understanding of signaling and ligand binding mechanism via molecular dynamic simulations.
- **Research Associate** 2014 - 2015
  Department of Biosciences, Comsats University *Islamabad, Pakistan*
  - Worked on protein modeling, molecular docking, and MD simulations of bacterial proteins.
- **Research Assistant** 2013 - 2014
  National center for Bioinformatics, Quaid-i-Azam University *Islamabad, Pakistan*
  - Worked on projects mainly focusing on identification of resistant proteins in bacterial genome and virtual screening to identify potential vaccine or a drug candidate against those resistant species. I also worked on comparison of docking software such as GOLD, Autodock, and MOE.

Education

- **Ph.D. Computational Biology** 2015 – 2020
  Department of Molecular Science and Technology, Ajou University *Suwon, South Korea*
- **MPhil Bioinformatics** 2012 – 2014
  National center for Bioinformatics, Quaid-i-Azam University *Islamabad, Pakistan*
- **BS Bioinformatics** 2007 – 2011
  Department of Bioinformatics, GC University *Faisalabad, Pakistan*

Skills

- Proficient in computational design tools (MOE, PyMOL, Chimera, Schrodinger Suite).
- Proficient in molecular dynamic simulation tools (AMBER and GROMACS).
- Proficient in molecular docking and virtual screening tools (MOE, GOLD, Openeye, Autodock vina).
- Experience of R, PERL, and python.
- Experience of KNIME, TensorFlow, and Scikit.

Publications

- Nasir Javaid, Mahesh Chandra Patra, Da-Eun Cho, **Maria Batool**, Yoongeun Kim, Gwang Muk Choi, Moon Suk Kim, Dae-Hyun Hahm, Sangdun Choi (2022). An orally active, small-molecule TNF inhibitor that disrupts the homotrimerization interface improves inflammatory arthritis in mice. Science Signaling.
- Mariya Farooq, **Maria Batool**, Moon Suk Kim, Sangdun Choi (2022). Toll-like receptors as a therapeutic target in the era of immunotherapies. Frontiers in Cell and Developmental Biology.
- Ahmad B, **Batool M**, Ain QU, Choi S (2021). Exploring the binding mechanism of PF-07321332 SARS-CoV-2 protease inhibitor through molecular dynamics and binding free energy simulations. International Journal of molecular sciences 22(17), 9124.
- **Batool M**, Kim MS, and Choi S (2021). Structural insights into the distinctive RNA recognition and therapeutic potentials of RIG-I-like receptors. Medicinal Research Reviews. 1- 27.
- Pirzada RH, Haseeb M, **Batool M**, Kim MS, and Choi S (2021). Remdesivir and Ledipasvir among the FDA-Approved Antiviral Drugs Have Potential to Inhibit SARS-CoV-2 Replication. Cells, 10(5).
- Ahmad B, **Batool M**, Kim MS, and Choi S (2021). Computational-Driven Epitope Verification and Affinity Maturation of TLR4-Targeting Antibodies. International Journal of Molecular Sciences, 22(11).
- Patra MC, **Batool M**, Haseeb M, and Choi S (2020). A computational probe into the structure and dynamics of the full-length Toll-like receptor 3 in a phospholipid bilayer. International Journal of molecular sciences, 21(8).
- Ain QU, **Batool M**, and Choi S (2020). TLR4-Targeting Therapeutics: Structural Basis and Computer-Aided Drug Discovery Approaches. Molecules, 25(3), 627.
- **Batool M**, Ahmad B, and Choi S (2019). A structure-based drug discovery paradigm. International journal of molecular sciences 20 (11), 2783.
- Patra MC, Kwon HK, **Batool M**, and Choi S (2018). Computational insight into the structural organization of full-length Toll-like receptor 4 dimer in a model phospholipid bilayer. Frontiers in immunology 9, 489.
- **Batool M** and Choi S (2017). Identification of druggable genome in staphylococcus aureus multidrug resistant strain. IEEE Life Sciences Conference (LSC), 270-273.
- Yesudhas D, **Batool M**, Anwar MA, Panneerselvam S, Choi S (2017). Proteins Recognizing DNA: Structural Uniqueness and Versatility of DNA-Binding Domains in Stem Cell Transcription Factors. Genes 8 (8), 192.
- **Batool M**, Shah M, Patra MC, Yesudhas D, Choi S (2017) Structural insights into the Middle East respiratory syndrome coronavirus 4a protein and its dsRNA binding mechanism. Scientific Reports 7.
- **Batool M**, Anwar MA, Choi S (2016) Toll-Like Receptors Targeting Technology for the Treatment of Lymphoma. Expert Opinion and Drug Discovery 11 (11): 1047-1059.

- Durai P, **Batool M**, Shah M, Choi S (2015) Middle East respiratory syndrome coronavirus: transmission, virology and therapeutic targeting to aid in outbreak control. Experimental & molecular medicine 47 (8).
- Durai P, **Batool M**, Choi S (2015) Structure and Effects of Cyanobacterial Lipopolysaccharides. Marine Drugs 13 (7): 4217-4230.
- Azam SS, Abbasi SW, **Batool M** (2013) Structure modeling and docking study of HCV NS5B-3a RNA polymerase for the identification of potent inhibitors. Medicinal Chemistry Research 22(7): 3049-3540.
- **Batool M**, Khalid MH, Hassan MN, Hafeez FY (2011). Homology modeling of an antifungal metabolite plipastatin synthase from the Bacillus subtilis 168. Bioinformation 7(8).
- Butt AM, **Batool M**, Tong Y (2011). Homology modelling, comparative genomics and functional annotation of Mycoplasma genitalium hypothetical protein MG_237. Bioinformation 7(6).

Patent Applications

- Choi S, Hahm DH, **Batool M**, Patra MC, Javaid N, A novel small molecule inhibitor of Tumor necrosis factor alpha (TNF-α) (10-2019-014-132, KR) (Nov, 2019).

Awards and Honors

Global Scholarship, 2019-2020
Brain Korea (BK21) Fellowship, 2015-2018
Merit-based Fellowship, 2012-2014

References

Available upon request.