Melike Berksöz, PhD

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Education

- PhD, Molecular Biology and Bioengineering | Sabancı University, Turkey | 2018-2024
- M.Sc, Chemistry | Albert Ludwigs University of Freiburg, Germany | 2011-2014
- B.Sc, Chemistry | Middle East Technical University, Turkey | 2004-2010

Research Experience

PhD candidate | Sabancı University, Turkey | 2018-2024

- Investigated the allosteric regulation of fluorescence in protein-based biosensors with classical and enhanced molecular dynamics simulations.
- Performed Perturbation Response Scanning (PRS) to identify allosteric sites most suitable for insertion of reporter domains.
- Employed Alphafold2 with a focus on obtaining alternative conformations.
- Designed and ranked binding site and allosteric mutants in terms of ligand affinity using steered-MD simulations. Results are complemented by wet-lab experiments.

Research Scientist | İlko Pharmaceuticals, Teknopark İstanbul | 2016-2021

- Worked as an industrial PhD candidate in colloboration with Sabancı University.
- Involved in tech transfer from South Korean partner company Genexine.
- Developed liquid chromatography-mass spectrometry methods for characterization of therapeutic antibodies from mammalian expression systems; identified post-translational modifications including glycans, charge variants, disulfide shuffling, aggregation and stability.

Research Assistant | Albert Ludwigs University of Freiburg, Germany | 2011-2014

- Purified the ammonium transporter Amt1 and performed electrophysiology and Cryo-TEM to quantify the electrogenic ion current per monomer.

Publications

- **Berksoz, M.,** & Atilgan, C. (2024). Ranking single fluorescent protein based calcium biosensor performance by molecular dynamics simulations- *J. Chem. Inf. Model.* , 2024, https://doi.org/10.1021/acs.jcim.4c01478
- **Berksoz, M.,** & Atilgan, C. (2024). Allosteric modulation of fluorescence revealed by hydrogen bond dynamics in a genetically encoded maltose biosensor. *Proteins,* 92(8), 923–932. https://doi.org/10.1002/prot.26688
- Barakat, S., **Berksoz, M.,** Zahedimaram, P., Piepoli, S., & Erman, B. (2022). Nanobodies as molecular imaging probes. *Free Radical Biology & Medicine,* 182, 260–275. https://doi.org/10.1016/j.freeradbiomed.2022.02.031
- Gurel, B., **Berksoz, M.** et al (2022). Structural and Functional Analysis of CEX Fractions Collected from a Novel Avastin Biosimilar Candidate and Its Innovator: A Comparative Study. *Pharmaceutics*, 14(8), 1571. https://doi.org/10.3390/pharmaceutics14081571

Awards

- Travel grant - Bioexcel Summer School on Biomolecular Simulations, 2024, Sardegna, Italy
- Travel grant - European Biophysical Societies Association (EBSA) Congress, 2023, Stockholm, Sweden
- Biannual performance-based scholarship by Scientific and Technological Research Council of Turkey (TUBITAK) - awarded for two consecutive years

Skills & Expertise

Computational skills

- MD simulations and trajectory analysis; classical and biased MD-well-tempered metadynamics, steered molecular dynamics simulations and free energy calculations.
- MD input preparation; Alphafold/Colabfold, CHARMM-GUI (membrane builder, ligand modeler, PDB manipulation), topology modifications for ligands and non-standard amino acids (CHARMM36).
- Molecular visualization; VMD, Pymol, ChimeraX.
- HPC infrastructure; workload managers (slurm), Bash and the Unix command line.
- Data analysis workflows with Python notebooks (Jupyter, Colab).
- Data analysis and visualization with Graphpad Prism and Python libraries.

Experimental skills

- Recombinant protein production, reconstitution of membrane proteins into proteoliposomes and assessment of electrogenic ion transport with solid supported membrane based-electrophysiology.
- Biophysical characterization of therapeutic antibodies by liquid chromatography-mass spectrometry methods. Assessment of antibody-antigen interaction with Surface Plasmon Resonance Spectroscopy.
- Size-exclusion, Reverse-phase and cation exchange chromatography coupled with UV-VIS and mass detection (Q-ToF).
- Forced degradation study design and execution. Investigation of degradation pathways (deamidation, oxidation, thermal and pH stability).
- Capillary Electrophoresis- cIEF and CE-SDS, analysis of charge and clipping variants.

Teaching Experience

- Co-supervisor in EuroCC Project 'Navigating Energy Surface of Functional Proteins'.
- Teaching assistant for 'Structure and Function of Biological Macromolecules' course for two semesters- hands-on teaching VMD/NAMD, linux/HPC/terminal usage.
- Supervised a total of six undergraduate students over two summer internships - protein visualization, MD simulations and analysis software.
- Instructor for the EuroCC workshop 'Computational Design of Fluorescent Biosensors"

Selected Conference Proceedings

- **Berksoz M** and Atilgan C, Conformational Dynamics of Genetically Encoded Fluorescent Biosensors, *Bioexcel Summer School on Biomolecular Simulations*, 2024, Sardegna, Italy (poster presentation)
- **Berksoz M.** Çetin E., Atilgan C, Hydrogen Bond Dynamics in Genetically Encoded Fluorescent Biosensors, *European Biophysical Societies Association Congress*, 2023, Stockholm, Sweden (poster presentation)
- Atılgan C, Liu G., Jalalypour F., Ekmen E., **Berksoz M,** Atılgan A.R, Sayers Z., Increased ionic strength triggers multiple conformations in both apo and holo forms of bacterial ferric binding protein, February 2023, *Biophysical Journal* 122(3):444a-445a DOI: 10.1016/j.bpj.2022.11.2399 (contributed talk)

Languages

- Turkish (native), English (fluent), German (intermediate)

Referees

Prof. Canan Atılgan (thesis advisor)
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