# Melike Berksöz, PhD

mberksoz@sabanciuniv.edu +90 531 575 9001 midst.sabanciuniv.edu www.linkedin.com/in/melike-berksöz

# **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/10.1101/2024.07.29.605619
- **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 semestershands-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)

Sabancı University, İstanbul-Turkey e-mail: canan@sabanciuniv.edu phone: +90 216 483 95 23

# Dr. Huriye Erdogan Dagdas (former colleague)

MSAT Analytical Development-Protein Lead MeiraGTx, London-United Kingdom e-mail: huriye.dagdas@meiragtx.com phone: +44 020 3866 4320

# Prof. Batu Erman (thesis committee member)

Acıbadem University, İstanbul-Turkey e-mail: batu.erman@acibadem.edu.tr phone: +90 216 500 4318

# Dr. Başak Özata (former colleague)

Innovation Management Office German Cancer Research Center (DKFZ) e-mail: basak.oezata@dkfz-heidelberg.de