Berke Türkaydin

Computational Drug Discovery Scientist | Protein Dynamics & Structure-Based Design

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PROFESSIONAL SUMMARY

Computational Drug Discovery Scientist with 6+ years of experience on molecular simulations, protein design, and experimental validation. Consistently served as the sole computational lead across 4 international institutions, bridging experimental physiology, structural biology, and computational chemistry by translating high-dimensional simulation data into clear, testable hypotheses that drive experimental drug discovery decisions. Expert in scaling physics-based workflows, ML-assisted hit-to-lead optimization, and reducing experimental burden through high-confidence candidate prioritization.

PROFESSIONAL EXPERIENCE

Computational Drug Discovery Scientist — PhD Fellow | Leibniz-Molecular Pharmacology Institute (FMP Berlin) | *Sep 2021 – Present*

- **Structure-Based Modeling**: Designed and executed 50+ microsecond of GPU-accelerated MD and enhanced sampling across 20+ systems to characterize membrane protein systems for mechanism-driven drug discovery.
- **Protein Design:** Generated refined structural models using AlphaFold, Rosetta (RFdiffusion), and ProteinMPNN to provide testable hypotheses for downstream experimental validation.
- **Hit Identification:** Drove 2 drug hits currently in vivo testing by reducing 50,000 compounds to 20 prioritized candidates via virtual screening, docking (AutoDock, DiffDock), and MM-GBSA.
- **ML & Data Automation:** Developed custom PyTorch and RDKit pipelines for molecular descriptor filtering and tICA/MSM-inspired analysis to extract mechanistic trends from massive MD trajectories.
- **HPC Strategy:** Secured 350,000 GPU/CPU hours through 7 competitive proposals at national supercomputing centers in Germany and Switzerland
- **Coding & Programming:** Analyzed large-scale simulation pipelines in Python, enabling consistent, scalable post-processing and statistical evaluation of massive MD trajectories.
- **Leadership:** Served as sole computational lead coordinating 4 international institutions; mentored Master’s and PhD students while translating complex data for cross-functional collaborators.

Research Assistant | Leibniz-Molecular Pharmacology Institute (FMP Berlin) | *Nov 2019 – Jan 2021*

- Conducted MD simulations and non-standard residue parameterization to model experimentally observed bridging interactions in membrane proteins, supporting mechanistic interpretation.
- Investigated regulatory mechanisms and substrate recognition of insulin-degrading enzymes.

TECHNICAL SKILLS

Core Expertise & Drug Discovery

- **Simulations and Modeling:** GROMACS, AMBER, PLUMED, OpenMM, MD, Enhanced Sampling (Metadynamics, OPES)
- **Structure-based Design:** AutoDock, DiffDock, MM-GBSA, SBDD, Virtual Screening, Hit-to-Lead Optimization
- **Protein Engineering:** AlphaFold, Rosetta (RFdiffusion), ProteinMPNN, MODELLER, PyMOL, VMD, Blender

Machine Learning & Data Science

- **AI Frameworks:** PyTorch, scikit-learn, ML-assisted molecular descriptors (RDKit), dimensionality reduction (PCA, tICA), clustering, MSM-inspired analysis, application of autoencoders, latent space modeling
- **Data Analysis:** Python (NumPy, Pandas, SciPy), trajectory analysis, high-dimensional data processing, statistical analysis

Infrastructure & Automation

- **Workflow & HPC:** Linux-Unix Clusters, SLURM, PBS, GPU-accelerated workloads, Reproducible Analysis Pipelines, high-throughput simulation pipelines

EDUCATION

- **Ph.D. Structural Chemistry & Computational Biophysics** | Technische Universität Berlin | Sep 2021 – Present
- **M.Sc. Biochemistry** | Freie Universität Berlin | Apr 2018 – Sep 2021
- **B.Sc. Molecular Biology & Genetics** | Istanbul Technical University | Sep 2012 – Jan 2018

SELECTED PUBLICATIONS

- **Türkaydin, B. et al. (2026)** *Energetic cross-talk of filter gate and lower helices drives polymodal regulation and disease in TREK K2P Channels*. In review - **Nature Communications**
- **Türkaydin, B. et al. (2024)** *Atomistic mechanism of coupling between cytosolic sensor domain and selectivity filter in TREK K2P channels*. **Nature Communications**
- Google Scholar

LANGUAGES & PERSONAL

- **Languages:** English (C1), German (B2), Turkish (Native)
- **Civics:** Dual Citizenship (German/Turkish)
- **Leadership:** National Fencing Athlete (2010–2019), represented Turkey in international competitions.
- **Awards:** From PhD to Innovator Certificate (2024), FEBS Youth Travel Fund Grant (2022)
- **Technical:** Linux/Unix, Python, Jupyter Notebook, https://github.com/BerkeTurkaydin

Extended CV