Emre Taha Çevik

MSc student in Bioinformatics & Systems Biology · molecular dynamics, cryptic and allosteric pockets, AI-based structure prediction

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EDUCATION

MSc, Bioinformatics and Systems Biology 02/2025 – 06/2027 (expected)
Gebze Technical University, Türkiye · taught in English
GPA 3.43/4.00 · Thesis: *Molecular Modeling and Machine Learning Approaches for Neoantigen Prediction* · Supervisor: Dr. Onur Serçinoğlu

BSc, Bioengineering 09/2019 – 02/2025
Gebze Technical University, Türkiye · taught in English
GPA 2.96/4.00 · TÜBİTAK 2209-A undergraduate research project (see below)

RESEARCH EXPERIENCE

PocketHunter: pocket detection across molecular dynamics trajectories 09/2023 – present
Gebze Technical University · Supervisor: Dr. Onur Serçinoğlu · TÜBİTAK 2209-A (09/2023 – 12/2024), continued in MSc

- Lead developer of **PocketHunter** (github.com/costbio/PocketHunter), a command-line pipeline that extracts frames from MD trajectories, predicts pockets per frame (P2Rank) and clusters them to characterise druggable and cryptic binding sites.
- Built **PocketHunter Suite** (github.com/costbio/PocketHunter-Suite), a public web platform combining the pipeline with SMINA docking and a Mol* 3D viewer; containerised workers, job orchestration, PostgreSQL and CI for multi-user deployment.
- Manuscript in preparation for the *Nucleic Acids Research* Web Server Issue 2027.

AI-based structural modelling of peptide–MHC complexes for neoantigen assessment 08/2025 – present
TÜSEB strategic R&D project (Health Institutes of Türkiye, Turkish Cancer Institute), building a neoantigen discovery platform for mRNA cancer vaccines · Role: project scholarship holder · PI: Prof. Dr. Uygar H. Tazebay

- Built a workflow to predict peptide–MHC complexes with deep-learning structure predictors (Chai-1, Boltz-2), rank candidate models and validate binding-groove conformations against known structures.
- Ran and analysed replicated MD simulations of predicted complexes (AMBER/GROMACS) and benchmarked predictors against experimental structures; independently explored binding free-energy estimates (MM/PBSA). Manuscript expected.
- On my own initiative, built tools to scale the simulation work: **mdkit**, reproducible post-MD analysis across complexes × replicas, and **gmx-watchtower**, monitoring and management of GROMACS job queues (github.com/bogrum/mdkit).

Allosteric inhibitor discovery for full-length PTP1B (type 2 diabetes) 09/2025 – 06/2026
BSc graduation project, Gebze Technical University · Supervisors: Assoc. Prof. Abdülkadir Koçak, Prof. Dr. Tunahan Çakır · Role: MD lead and mentor

- Ran most of the molecular dynamics: AlphaFold3 model of full-length PTP1B, vacuum pre-folding of the extended C-terminal tail, 5 × 1 µs production replicas (GROMACS, AMBER99SB-ILDN).
- Trained the student in trajectory clustering, multi-method allosteric pocket detection and an HPC docking campaign on TRUBA (1.77 M compounds, SMINA, SLURM array jobs).

Research scholar, TÜBİTAK 3501 career development project 08/2023 – 10/2023
Alparslan Türkeş Science and Technology University · Supervisor: Assoc. Prof. Yeliz Gürdal Durğun

- H_2 production mechanisms of cobalt-based water-reduction catalysts with ab initio MD, DFT and free energy perturbation.

Independent computational projects 2025 – 2026

- Systematic GROMACS 2025.3 GPU benchmark on the national TRUBA HPC cluster (~600 runs over MPI/OpenMP/GPU settings; best 228 ns/day) to size the lab's simulation campaigns (repo).
- Seminar project: reproduced Weber *et al.* (2024) on MD-derived features for MHC-I peptide immunogenicity and tested a graph convolutional network in PyTorch (repo).

Co-founder, pHelix (early-stage bioinformatics start-up) 09/2026 – present

Building a pay-as-you-go cloud platform for clinical exome analysis: nf-core/sarek on AWS Batch, VEP annotation, multi-tenant data isolation, usage metering and billing; main developer of the pipeline and infrastructure.

Research internships 2023 – 2024

ERA Pharma, İstanbul (06–07/2024) · GTU Bioinformatics Laboratory (07–08/2023): data mining of protein–ligand pairs and front-end development for a bioinformatics tool.

CONFERENCE PRESENTATIONS

Çevik ET. Development of a web-based tool for identification of druggable pockets in protein conformational ensembles and ensemble docking. Oral presentation, *HIBIT 2024, International Symposium on Health Informatics and Bioinformatics*, Bezmialem Vakıf University, İstanbul, Türkiye, 19 December 2024.

MANUSCRIPTS IN PREPARATION

Çevik ET, Serçinoğlu O, *et al.* PocketHunter: tracking binding pockets across molecular dynamics ensembles. Target: *Nucleic Acids Research* Web Server Issue 2027.

SKILLS

Simulation	GROMACS and AMBER (system setup, replicated production runs, trajectory analysis), ab initio MD and DFT (research training), Monte Carlo (RASPA), free-energy concepts
Structure & design	Chai-1, Boltz-2, AlphaFold 3, PANDORA; docking (SMINA, AutoDock Vina); P2Rank; MM/PBSA (gmx_MMPBSA); PyMOL, VMD, Mol*
Programming	Python (scientific stack, CLI and web tools), Bash, Linux/HPC, Git/GitHub (pull-request workflow, CI), Docker, Streamlit, PostgreSQL; basic HTML/CSS/JavaScript
Languages	Turkish (native) · English (C1; both degrees taught in English)

LEADERSHIP & SERVICE

Member, ISCB Student Council (international) 10/2026 – present

Joined on invitation from the Student Council leadership.

President, ISCB Student Council Regional Student Group Türkiye (RSG-Türkiye) 01/2026 – present

- Led and built the group's bilingual (TR/EN) web platform (rsg-turkiye.iscbsc.org; 500+ commits, 250+ pull requests): member accounts, learning paths, an archive of 80+ webinars, certificate verification and a content system with approval workflow, so the community keeps running across leadership changes.
- Organising team of three national student symposia: coordinated the 13th (Ankara, Middle East Technical University, October 2026) and co-organised the 12th (2025, HIBIT 2025 satellite) and 11th (2024, Istanbul).
- Organised RSG-Türkiye local sites of the nf-core hackathon (March 2025 and March 2026, İstanbul), with contributions merged into nf-core pipelines.
- Earlier roles: Secretary (2025; *Dock'n Roll* molecular docking hackathon with YTÜ BİYOGEN), journal-club member (2023–2025).

Teaching & student clubs 2022 – 2023

Instructor, Deneyap Türkiye (CAD design for middle-school students) · Board member and head of the theoretical biology committee, GTU IAPS student club.

GRANTS & SCHOLARSHIPS

TÜSEB research project scholarship (peptide–MHC modelling project) 08/2025 – present

TÜBİTAK 2209-A Undergraduate Research Project Grant 2023 – 2024

TÜBİTAK 3501 Career Development Programme, research scholarship 2023

REFERENCES

Available on request.