ÖZDE ZEYNEP GÜNER-YILMAZ

PhD in Chemical Engineering

ORCID | Google Scholar | GitHub

EDUCATION

Ph.D. in Chemical Engineering 2026
Istanbul Technical University (İTÜ), Istanbul, Turkey | GPA: 3.86/4.00

- Thesis: Development of Two Network Models for Investigating Conformational Dynamics and Allosteric Mechanisms in Protein Complexes for Structure-Based Drug Design
- Developed MCG-ANM, a mixed coarse-grained elastic network model for conformational sampling and ensemble docking.
- Developed MUSIKALL, a k-shortest path algorithm tool using residue interaction networks for allosteric communication analysis.

M.Sc. in Biomedical Engineering 2020
Boğaziçi University, Istanbul, Turkey | GPA: 3.75/4.00

- Thesis: Functionalization of Carbon Nanotubes as Drug Carriers in Cancer Treatment
- Synthesized Fmoc–PEG functionalized single-walled carbon nanotubes; characterized dispersibility and cytocompatibility for cancer drug delivery.

B.Sc. in Chemical Engineering 2018
Istanbul Technical University (İTÜ), Istanbul, Turkey

- Capstone Project: Multi-Scale Investigation of Pectin–Drug Systems Using Computational and Experimental Methods

RESEARCH EXPERIENCE

Researcher Feb 2026 – Present
BIND Lab (Bionanotechnology & Nanomedicine Lab, Max Planck Partner Group), Boğaziçi University

- TÜBİTAK 1004 Project (No. 23AG005): Neurotechnological solutions platform — developing magnetic biomaterial and nanoparticle platforms for neurotechnology applications.

Doctoral Researcher 2021 – 2026
Computational Structural Biology Lab, Istanbul Technical University (Advisor: Assoc. Prof. Özge Kürkçüoğlu Levitas)

- TÜBİTAK 1002 (No. 125Z132): Developed and validated MUSIKALL, a software for k-shortest path based allosteric pathway analysis in proteins. Applied to GPCR and enzyme systems.
- TÜBİTAK 1004 / NANOSIS (No. 20AG029): Developed nanoparticle-integrated multifunctional wound dressings; hydrogel–nanoparticle hybrid matrices; sensor platform for wound monitoring (2021–2025).
- ITU-BAP ILAP 3 Project: Designing injectable polysaccharide-based hydrogels for osteoarthritis treatment with rheological and computational characterization (2025–ongoing).
- ITU-BAP: Protein adsorption characterization of single-walled carbon nanotubes with varied surface chemistries; rheoloigcal evaluation in hydrogel matrices (2024).
- ITU-BAP: Structure-based drug design using mixed-resolution elastic network model; MCG-ANM conformer generation for docking and binding free energy calculations (2021–2026).

Industry Collaboration 2020
BSH — Preparation and Characterization of Antibacterial Composites

- Developed polypropylene-based composite materials with modified zeolite additives.

SOFTWARE TOOLS DEVELOPED

MCG-ANM Published in JCIM 2025

- A computationally efficient mixed coarse-grained anisotropic network model for conformational sampling, ensemble docking, and binding free energy calculations.

MUSIKALL TÜBİTAK 1002 Funded

- A k-shortest path algorithm platform built on residue interaction networks (RIN) for mapping allosteric communication pathways and identifying long-range signaling mechanisms in proteins.

PUBLICATIONS

1. Güner-Yılmaz, Ö.Z., Kocaaga, B., Yılmaz, A., Balcik, M., Kurkcuoglu, O., et al. Graphene Oxide-Based and Porous Nanocarriers for Drug Delivery Developed with Computational and Experimental Approaches. Surf. Interfaces, 107860 (2025).
2. Güner-Yılmaz, Ö.Z., Doruker, P., Kurkcuoglu, O. A Computationally Efficient Method to Generate Plausible Conformers for Ensemble Docking and Binding Free Energy Calculations. J. Chem. Inf. Model. 65(15), 8137–8157 (2025).
3. Aydın, B., Güner-Yılmaz, Ö.Z., Yılmaz, A., Kilic-Cevirgel, S., et al. Mitoxantrone release from Fmoc-protected amino acids coated magnetic carbon nanotubes: Computational and experimental study for cancer treatment. J. Drug Deliv. Sci. Technol. 101, 106291 (2024).
4. Kocaaga, B., Öztürk, Y., Kurçin, H.C., Güner-Yılmaz, Ö.Z., et al. Developing multifunctional pectin-based hydrogel for wound dressing: In silico, in vitro, and in vivo evaluation. Eur. Polym. J. 216, 113280 (2024).
5. Güner-Yılmaz, Ö.Z., Yılmaz, A., Bozoglu, S., et al. Single-walled (magnetic) carbon nanotubes in a pectin matrix in the design of an allantoin delivery system. ACS Omega 9(9), 10069–10079 (2024).
6. Güner-Yılmaz, Ö.Z., Kurkcuoglu, O., Akten, E.D. Tunnel-like region observed as a potential allosteric site in Staphylococcus aureus Glyceraldehyde-3-phosphate dehydrogenase. Arch. Biochem. Biophys. 752, 109875 (2023).
7. Güner, O.Z., Kocaaga, B., Batirel, S., Kurkcuoglu, O., Guner, F.S. 2-Thiobarbituric Acid Addition Improves Structural Integrity and Controlled Drug Delivery of Biocompatible Pectin Hydrogels. Int. J. Polym. Mater. Polym. Biomater. 70(10), 703–711 (2021).

GRANTS & AWARDS

TÜBİTAK 1004 Doctoral Research Fellowship (No. 23AG005) — Feb 2026 – Present

TÜBİTAK 1002 Research Grant (No. 125Z132) — MUSIKALL — Sept 2025 – Dec 2025

TÜBİTAK 2224-A International Scientific Events Grant — 2025

ITU BAP Advanced Research Project Doctoral Fellowship — Feb 2025 – Sept 2025

TÜBİTAK 2250 Graduate Performance Fellowship — 2024/2 & 2025/1

YÖK 100/2000 Priority Areas Doctoral Fellowship — May 2021 – Mar 2025

TÜBİTAK 1004 Doctoral Research Fellowship / NANOSIS (No. 20AG029) — Mar 2021 – Feb 2025

TÜBİTAK 1004 Undergraduate Research Fellowship — Jul – Nov 2017

SELECTED CONFERENCE PRESENTATIONS

- Güner-Yılmaz, Ö.Z., Doruker, P., Kurkcuoglu, O. Use of a Mixed-Resolution Elastic Network Model in Binding Free Energy Calculations. [Oral] 18th International Symposium on Health Informatics and Bioinformatics, Istanbul, Turkey, Oct 2025.
- Güner-Yılmaz, Ö.Z., Duranlar, Ö., Çetin, S., Guner, F.S. Influence of 2-thiobarbituric acid on the structural and rheological properties of injectable hydrogels. [Poster] European Polymer Congress (EPF 2025), Groningen, Netherlands, Jun 2025.
- Güner-Yılmaz, Ö.Z., Memişoğlu, İ.G., et al. Biochar as a sustainable carrier: Effect of procaine loading and BSA coating. [Oral] 16th National Chemical Engineering Congress, Bolu, Turkey, Sept 2025.
- Güner-Yılmaz, Ö.Z., Alp, C.N., Kurkcuoglu, O. A computational tool for predicting information flow in proteins using k-shortest path algorithm. [Poster] 35th National Chemistry Congress, Diyarbakır, Turkey, Sept 2024.
- Güner-Yılmaz, Ö.Z., Kurkcuoglu, O. Use of Truncated Structures in Molecular Dynamics Simulations for Investigating Protein–Ligand Interactions: A Case Study on Triosephosphate Isomerase. [Poster] ISQBP President's Meeting, Athens, Greece, May 2024.

SCHOOLS & WORKSHOPS

- European Society for Biomaterials: Alpine Winter School for Biofabrication, Radstat, Austria, Jan 2026
- MIDST: Modeling Membrane-Embedded Proteins and Ligand Transport, Sabancı University, Istanbul, Dec 2025
- Exploring Biomolecular Modeling and Simulations — EuroCC4SEE & BioExcel, Online, Apr 2025
- MIDST: Mapping the Protein Landscape with Metadynamics, Sabancı University, Istanbul, Mar 2024
- EMBO Practical Course — Integrative Modelling of Protein Interactions, Izmir, Turkey, Sept 2023
- EMBO Workshop: Advances and Challenges in Biomolecular Simulations, Online, Oct 2021

TECHNICAL SKILLS

Computational Methods & Software

MD Simulation: NAMD, Desmond (Schrödinger Maestro) — trajectory preparation and analysis

Elastic Network Models: MCG & ANM — conformer generation, normal mode analysis

Allostery & Networks: Residue Interaction Network (RIN) + k-shortest path algorithm — allosteric pathway identification and intramolecular communication mapping

Molecular Docking: AutoDock Vina; Glide XP (Schrödinger Maestro) — multi-conformer docking, binding mode analysis; MM/GBSA binding free energy

Materials Modeling: Materials Studio (Adsorption Locator, MD, Quench) — polymer–drug interactions, carbon material modeling, adsorption energy and surface interaction analysis

Visualization: PyMOL, ChimeraX, VMD, Discovery Studio Visualizer

Bioinformatics: Jalview, UniProt, GPCRdb, PDB Tools — sequence alignment, annotation, GPCR structural mapping

Programming: Python, MATLAB, GNU Octave — data processing, modeling, statistical analysis; SPSS

Other software: AutoCAD, CHEMCAD, Gaussian (basic), FORTRAN (basic)

Experimental Techniques

Rheology: Rotational rheometer — shear-thinning (G'/G"), creep-recovery, flow curves, self-healing

Tribology: Friction coefficient under load; lubrication and surface–material interactions at hydrogel interfaces

Spectroscopy & Surface: FTIR, UV–Vis spectrophotometry, BET surface area, contact angle goniometry

Particle Characterization: DLS — hydrodynamic size, zeta potential, and stability (nanoparticles and hydrogels)

Preparation: Lyophilization (freeze dryer), nanoparticle synthesis

Data Interpretation — Collaborative (evaluation and reporting expertise)

Morphology & Surface: SEM-EDS, surface roughness, wettability analysis

Mechanical & Thermal: Tensile strength, elongation, TGA, DSC — degradation and thermal stability

Magnetic & Elemental: VSM (nanoparticle magnetization); ICP-OES (Ca^{2+} release/adsorption, Fe content)

Cell-Based Assays: Viability, cytotoxicity, proliferation, scratch assay, hemolysis, wound healing, and drug delivery

Antioxidant Activity: DPPH radical scavenging — kinetic interpretation

LANGUAGES

Turkish: Native

English: Advanced — YOKDIL 90/100 (2025)

French: Upper-intermediate — DELF B2 Certificate

REFERENCES

Assoc. Prof. A. Özge Kürkçüoğlu Levitas
PhD Advisor — Chemical Engineering, Istanbul Technical University
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