Özde Zeynep Güner Yılmaz

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RESEARCH OUTPUT SUMMARY

I am a PhD candidate in Chemical Engineering at Istanbul Technical University, specializing in computational structural biology and biomaterials. I am supported by the YÖK 100/2000 Scholarship, a national doctoral program designed to train researchers in prioritized scientific fields.

My PhD focuses on the computational investigation of drug-protein interactions, protein conformational dynamics, and intra-protein communication. In parallel, I have contributed to biomaterials projects, where we developed injectable, biocompatible hydrogels and nano-carrier systems for controlled drug delivery and tissue repair. My long-term research interest centers on understanding how drugs behave within proteins, materials, and biological interfaces, and using this knowledge to design more effective therapeutic delivery systems.

EDUCATION

Istanbul Technical University, GPA:3.86/4.00 — Istanbul, Türkiye
PhD, Chemical Engineering — 2020-Ongoing
Research Focus: Developing a computational method that integrates Mixed Coarse-Graining and Anisotropic Network Model to efficiently explore protein conformations and calculate binding free energy. Using k-shortest path algorithms and residue interaction networks to analyze how distant residues communicate and to identify potential allosteric sites.

Boğaziçi University, **GPA:3.75/4.00** — Istanbul, Türkiye
MSc, Biomedical Engineering — 2018-2020
Thesis: Functionalization of Carbon Nanotubes for Drug Delivery in Cancer Therapy
Designed and synthesized Fmoc–PEG functionalized single-walled carbon nanotubes, improving their aqueous dispersibility and cytocompatibility, and experimentally validated their potential as nanocarriers for cancer drug delivery.

Istanbul Technical University — Istanbul, Türkiye
BSc, Chemical Engineering — 2015-2018
Graduation Project: A Multiscale Investigation on Pectin-Drug Systems by Molecular Dynamics Simulation and Experimental Methods

HONORS AND SCHOLARSHIPS

- TÜBİTAK 1002 Project Research Scholarship — Sept. 2025 - Ongoing
- TÜBİTAK 2224-A Support Program for Participation in International Scientific Events — 2025/1
- ITU BAP* Scholarship — Feb. 2025 - Sept. 2025
- YÖK** 100/2000 Priority Area Ph.D. Scholarship — May. 2021 - Mar. 2025
- TÜBİTAK*** 1004 Project – NANOSIS (20AG029) — Mar. 2021 - Feb. 2025
- TÜBİTAK*** 2250 – Graduate Scholarship Performance Program — Feb. - Jul. 2024
- TÜBİTAK*** 1004 Project Research Scholarship — Jul. – Nov. 2017

RESEARCH EXPERIENCE

ITU-BAP*

- **ILAP 3 Project** — 2024-Ongoing
  Development of Injectable Hydrogels for Osteoarthritis Treatment
  Project-Funded Researcher

  Developing injectable polysaccharide-based hydrogels for osteoarthritis treatment by optimizing formulation parameters, crosslinking strategies, and additive incorporation. Conducting rheological analysis, swelling, degradation, and mechanical characterization to evaluate injectability and functional performance. In parallel, performing computational modeling including molecular interactions between hydrogel components, drug–material interfaces, and network-level behavior to guide rational design and enhance therapeutic efficiency.

- **Development of Hyaluronic Acid-Modified Hydrogel Formulations** — 2024, Ended
  Researcher

  Designed and characterized hyaluronic acid–enhanced hydrogel formulations, focusing on improved mechanical stability, water retention, and biomedical applicability.

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- **Investigation of Protein Adsorption Capacities and Performance of Single-Walled Carbon Nanotubes with Different Surface Chemistries** 2024, Ended
  Researcher

Examined the protein adsorption capacities and performance of single-walled carbon nanotubes with various surface modifications and performed rheological studies to analyze their flow properties and mechanical performance in hydrogels.

- **Application of Mixed Resolution Elastic Network Model in Structure-Based Drug Design** 2021-Ongoing
  Researcher

Developing a computationally efficient mixed-resolution modeling workflow to generate conformers for docking and molecular simulations, enabling large-protein/small-molecule interaction studies with reduced computational cost.

TÜBİTAK***

- **Development and Application of Software for Revealing Allosteric Mechanisms in Protein Structures Using the K-Shortest Path Algorithm** 2025, Ongoing
  TÜBİTAK 1002 Project (Project No:125Z132)
  Project-Funded Researcher

Developing a computational tool that identifies communication pathways in proteins using residue interaction networks and k-shortest path algorithms. Contributing to algorithmic refinement, software implementation, and validation on GPCRs and enzyme systems to detect allosteric hotspots and long-range signal propagation routes.

- **Development of Sensor-Integrated Wound Dressings for Monitoring and Treatment of Venous Ulcer** 2021-25, Ended
  TÜBİTAK 1004 Project (Project No: 20AG029)
  Project-Funded Researcher

Developed multifunctional wound dressings integrating nanoparticles for antimicrobial activity, drug loading–release, and moisture management. Designed hydrogel–nanoparticle hybrid matrices, optimized drug loading efficiency, and contributed to the development of a real-time sensing platform for monitoring wound healing.

Industry Collaborated Projects

- **BSH – Preparation and Characterization of Antibacterial Composites** 2020, Ended
  Researcher

Developed polypropylene-based composites using modified zeolite additives.

PUBLICATIONS

- **Güner-Yılmaz, Ö. Z.**; Kocaaga, B.; Yılmaz, A.; Balcik, M.; Kurkcuoglu, O.; Sungur, F. A.; Yavuz, R.; Karatepe, N.; Tatlier, M.; Sirkecioglu, A.; Hooshmand, S.; Aliari Miavaghi, M.; Ahmed Zabara, M.; Yürüm, A.; Bayazıt, M. K.; Batirel, S.; Güner, F. S. Graphene Oxide-Based and Porous Nanocarriers for Drug Delivery Developed with Computational and Experimental Approaches. (2025) *Surf. Interfaces*, 107860.
- **Güner-Yılmaz, Ö. Z.**, Doruker, P., Kurkcuoglu, A Computationally Efficient Method to Generate Plausible Conformers for Ensemble Docking and Binding Free Energy Calculations. (2025) *J. Chem. Inf. Model.* 65 (15), 8137–8157.
- Aydın B, **Güner-Yılmaz ÖZ**, Yılmaz A, Kilic-Cevirgel S, Karaoglu İC, Bozoglu S, İzbudak B, Kurkcuoglu O, Bal-Öztürk A, Karatepe N. Güner F.S. Mitoxantrone release from Fmoc-protected amino acids coated magnetic carbon nanotubes: Computational and experimental study for cancer treatment. (2024) *Journal of Drug Delivery Science and Technology*, 101, 106291, ISSN 1773-2247
- Kocaaga B, Öztürk Y, Kurçin HC, **Güner Yılmaz ÖZ**, Kurkcuoglu O, Tatlier M, Özdemir İ, Kervancioglu Demirci E, Kotil T, Solakoğlu S, Aksu B, Batirel S, Bal-Öztürk A, Güner FS. Developing multifunctional pectin-based hydrogel for wound dressing: In silico, *in vitro*, and *in vivo* evaluation. (2024) *European Polymer Journal*, 216, 113280.
- **Güner Yılmaz ÖZ**, Yılmaz A, Bozoglu S, Karatepe N, Batirel S, Sahin A, Güner FS. Single-Walled (Magnetic) Carbon Nanotubes in a Pectin Matrix in the Design of an Allantoin Delivery System (2024) *ACS Omega*, 9(9) 10069-10079.
- Murat FS, **Güner Yılmaz ÖZ**, Bozoglu S, Batirel S, Baysak, E, Hizal G, Karatepe N, Güner FS. (2024) Non-Covalent Functionalization of Magnetic Carbon Nanotubes with Fmoc Amino Acid-Modified Polyethylene Glycol, *ChemNanoMat*, 10(7).
- **Guner-Yılmaz OZ**, Kurkcuoglu O, Akten ED. Tunnel-like region observed as a potential allosteric site in Staphylococcus aureus Glyceraldehyde-3-phosphate dehydrogenase. (2023) *Arch. Biochem Biophys*. 752:109875.
- **Güner Yılmaz ÖZ**, Güner FS. Hyaluronic Acid-Enriched Pectin-Based Hydrogel Films for Wound Healing (2023) *ITU ARI-Bulletin of the Istanbul Technical University*, 55(1), Special issue: In memoriam to the late Prof. Dr. Yusuf Yağcı.
- Yeniyurt Y, Kilic S, **Güner-Yılmaz ÖZ**, Bozoglu S, Meran M, Baysak E, Kurkcuoglu O, Hizal G, Karatepe,N, Batirel S, Güner FS. Fmoc-PEG Coated Single-Wall Carbon Nanotube Carriers by Non-covalent Functionalization: An Experimental and

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Molecular Dynamics Study. (2021) *Frontiers in Bioengineering and Biotechnology*, 9,648366.

- **Guner OZ,** Kocaagaa B, Batirel S, Kurkcuoglu O, Guner FS. 2-Thiobarbituric Acid Addition Improves Structural Integrity and Controlled Drug Delivery of Biocompatible Pectin Hydrogels (2021*) International Journal of Polymeric Materials and Polymeric Biomaterials*, 70(10), 703-711.
- **Güner OZ**, Cam C, Arabacioglu-Kocaaga B, Batirel S, Güner FS, Theophylline-Loaded Pectin-Based Hydrogels: 1. Effect of Medium pH and Preparation Conditions on Drug Release Profile. (2018) *Journal of Applied Polymer Science*, 135(38) 46731.
- Erkal Ilhan S, Kürkçüoğlu Ö, Inan T, **Güner ÖZ**, Dalgakıran D, Okutan B, Torun Köse G, Kırmızı A, Okçu Heper A, Gürses Ö, Güner FS, Preparation and Determination of In Vivo and In Vitro Performance of Doxycycline Imprinted Contact Lenses for Corneal Neovascularization Treatment. (2018) *Journal of the Turkish Chemical Society, Section A: Chemistry*. 5(3), 1185-1192.

CONFERENCE PRESENTATIONS

- Using Mixed-Resolution Elastic Network Model for Binding Free Energy Calculations, 18th International Symposium on Health Informatics and Bioinformatics, İstanbul-Türkiye, Oct 2025
- Influence of 2-Thiobarbituric Acid on the Structural and Rheological Properties of Injectable Hydrogels, *European Polymer Congress (EPF 2025),* Groningen-Netherlands, Jun 2025.
- Sürdürülebilir Taşıyıcı Sistem Olarak Biyoçar: Prokain Yükleme ve BSA Kaplama Etkisi, *16th National Chemical Engineering Congress*, Bolu-Türkiye, Sept 2025.
- A Computer Program for Predicting Information Flow in Proteins Using k-Shortest Paths, *35th National Chemistry Congress*, Diyarbakır-Tükiye, Sept 2024.
- Using Truncated Structures in Molecular Dynamics Simulations to Investigate Protein-Ligand Interactions: A Case Study with Triose Phosphate Isomerase, *The International Society of Quantum Biology and Pharmacology President's Meeting*, Athens-Greece, May 2024
- Nanoparticle-Added Custom Design Wound Dressing: Potential Use of Graphene Oxide and Modified Graphene Oxide-Added Natural Hydrogels*, 15th National Chemical Engineering Congress,* Çanakkale-Türkiye, Sept 2023
- Investigating Potential Allosteric Communication Paths in S.aureus GAPDH using Residue Interaction Networks, *19th Asian Chemical Congress*, İstanbul-Türkiye, Jul 2023
- Mitoxantrone-Loaded Magnetic Single-Walled Carbon Nanotubes as Nanocarriers for Cancer Treatment, *Global Nanobio E-Conference*, Tampa-FL(online), Mar 2021
- Single-Walled Carbon Nanotube-added Pectin Hydrogels for Wound Dressing Applications, *14th National Chemical Engineering Congress*, Konya-Türkiye, Jun 2021
- Functionalization of carbon nanotubes for the use in cancer treatment, *3rd International Eurasian Conference on Biological and Chemical Sciences (EurasianBioChem 2020)*, Ankara-Türkiye, Mar 2020
- Synthesis of Thiolated Pectin-Based Drug Carrier Hydrogels with 2-Thiobarbituric Acid, *International Eurasian Conference on Biological and Chemical Sciences (EurasianBioChem 2018),* Ankara-Türkiye, Apr 2018
- Development of Sulfide-Bridged Pectin-Based Drug Carrier Hydrogels: Crosslinker Effect, *Advanced Polymers via Macromolecular Engineering (APME 2017),* Ghent-Belgium, May 2017
- Synthesis and Characterization of Pectin-Based Hydrogel Films: Effect of pH and Drug Loading Method on Drug Release Kinetics, *46th IUPAC World Polymer Congress (MACRO 2016)*, Istanbul-Türkiye, Jul 2016

WORKSHOPS

- Exploring Biomolecular Modeling and Simulations: EuroCC4SEE & BioExcel — Apr. 2025
- Dialogues in the MIDST Workshop: Mapping the Protein Landscape with Metadynamics — Mar. 2024
- EMBO Practical Course - Integrative modelling of protein interactions — Sep. 2023
- EMBO Workshop: Advances and Challenges in Biomolecular Simulations — Oct. 2021
- RSG Türkiye Computational Structural Biology Virtual Workshop — Dec. 2021
- Python for Data Science, Brock University Digital Scholarship Lab. — Sept. 2021
- Introduction to Python, Brock University Digital Scholarship Lab. — Sept. 2021
- Introduction to Python I – II – III – IV, Toronto Public Library Digital Innovation Hubs — Sept.-Oct. 2021

LANGUAGES

- Turkish: Native
- English: Advanced (YÖKDİL 90/100, 2025)
- French: Upper Intermediate (DELF B2 Certified)

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TECHNICAL & INSTRUMENTAL SKILLS

Experimental Techniques

- **Rotational Rheometer**: Shear-thinning behavior, viscoelastic properties (G', G''), creep–recovery analysis, flow curves, and self-healing performance of hydrogels and polymeric systems.
- **Tribological Characterization (Hydrogel & Soft Material Interfaces)**: friction coefficient evaluation, lubrication behavior, and surface-material interaction assessment under load
- **FTIR Spectroscopy**: Chemical structure and functional group characterization of polymers, hydrogels, and carbon-based materials
- **BET Surface Area Analysis**: Specific surface area and porosity measurements of nanocarriers and biochar
- **UV–Vis Spectrophotometry**: Quantitative analysis of drug loading, release kinetics, and adsorption behavior
- **Contact Angle Goniometry**: Surface wettability and interfacial property assessment
- **Freeze Dryer (Lyophilization):** Sample preparation for structural, morphological, and release studies

Solid Particle & Composite Material Analysis (Data-Level Competence)

Extensive experience interpreting experimental datasets generated by collaborators; proficient in scientific evaluation, problem-solving, and reporting.

- **Cell Culture Assays**: Interpretation of viability, cytotoxicity, proliferation, scratch assay, and hemolysis test data for wound healing and drug delivery studies.
- **DPPH Radical Scavenging Analysis**: Evaluation of antioxidant capacity results and kinetic interpretation.
- **Mechanical & Thermal Tests**: Interpretation of tensile strength, elongation, TGA, and DSC results for polymer and hydrogel systems, including degradation and thermal stability trends.
- **Surface & Morphology Analyses**: Data interpretation from SEM-EDS, and surface roughness/wettability assessments.
- **Magnetic & Surface Charge Analyses**: Evaluation of VSM, zeta potential, and DLS (hydrodynamic size distribution) results for nanoparticle and biochar-based systems.
- **Elemental Quantification**: Interpretation of ICP–OES data (Ca^{2+} release/adsorption, Fe-content assessment).

COMPUTATIONAL & SOFTWARE SKILLS

Structural Biology & Molecular/Materials Modeling

- **NAMD, Desmond (Schrödinger)**: Molecular dynamics simulations; trajectory preparation and analysis
- **Mixed Coarse-Graining (MCG) & Anisotropic Network Model (ANM)**: Conformer generation, normal mode analysis
- **Residue Interaction Networks & K-Shortest Path Algorithms**: Allosteric pathway detection and communication mapping
- **Materials Studio (Adsorption Locator, MD, Quench)**: Polymer–drug interactions, carbon material modeling, adsorption energy, and surface interaction analysis
- **AutoDock Vina; Glide XP**: Docking, ensemble docking, binding mode analysis
- **MM/GBSA**: Binding free energy calculations
- **PyMOL, ChimeraX, VMD, Discovery Studio Visualizer**: Structural visualization and figure preparation

Sequence & Bioinformatics Tools

- **Jalview, UniProt, GPCRdb, PDB Tools**: *Sequenc*e alignment, annotation, GPCR structural mapping

Programming & Data Analysis

- **Python, MATLAB, GNU Octave**: Data processing, modeling, statistical analysis
- **SPSS**: Statistical test interpretation and reporting

General Scientific & Engineering Software

- **AutoCAD**: Technical drafting and schematic design
- **CHEMCAD**: Basic process modeling and simulation
- **Gaussian (Basic Proficiency)**: Small-molecule optimization; introductory quantum chemical calculations
- **FORTRAN (Basic Proficiency)**: Reading and modifying legacy scientific scripts

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REFEREES

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