# Tandac Furkan Guclu

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## EDUCATION

**Sabanci University,** Istanbul, Turkey **2015 – 2021**
*PhD*, Molecular Biology, Genetics and Bioengineering
Thesis Subject: *Molecular Level Understanding of the Functionality of PDZ3 Variants via Advanced All-Atom Simulations and Dynamic Residue Network Analyses.*
Thesis Advisors: Dr. Canan Atilgan, Dr. Ali Rana Atilgan

**Marmara University,** Istanbul, Turkey **2013 – 2015**
*MSc*, Faculty of Engineering, Bioengineering
Thesis Subject: *Structural Dynamics of von Hippel-Lindau Tumor Suppressor Protein.*
Thesis Advisor: Dr. Asuman Nevra Ozer

**Hacettepe University,** Istanbul, Turkey **2007 – 2013**
*BSc,* Faculty of Science, Biology

## WORK EXPERIENCE

**Assistant Professor, İstinye University,** Istanbul, Turkey **2025 – present**
**Postdoctoral researcher, Sabanci University,** Istanbul, Turkey **2021 – 2025**

- Researcher at EuroCC4SEE (2024 – 2025)
- Researcher at EuroCC2 project (2023 – 2024)
- Researcher at EuroCC project (2022 – 2023)
- **Online open lectures:**
  - *Molecular Dynamics Simulations of Small Molecules* (View on Website).
  - *Prediction of Protein Structures Using Deep Learning Tools* (View on Website).
  - *Generating Mutant Protein Structures Using Advanced Techniques* (View on Website).
  - *Residue Networks: Understanding the Time Evolution and Mutations of Proteins from a Graph Theoretical Perspective* (View on Website).
- Co-lecturer of Computational Techniques for Materials at the Nano-scale (MAT 306), two semesters.
- Undergraduate projects (Program for Undergraduate Research (PURE)):
  Project Title: *Visual Assessment of AlphaFold2-Predicted Possible Transcytosis Protein Structures*. (with Dr. Nur Mustafaoğlu)
  Project Title: *DeepMind vs. Academia: How good are the best AI models in discriminating similar sequences of a given protein?* (with Dr. Canan Atilgan)
- Graduation project (ENS491 – ENS492):
  Project Title: *Temporal hydrogen-bond networks in proteins* (with Dr. Ali Rana Atilgan)

**Lecturer for School of Molecular and Theoretical Biology** **2024 (July – August)**

- Organized at Sabanci University, Turkey
- Taught high school and undergraduate students from various countries, including the USA, Japan, Russia, Ukraine, and Austria
- Delivered a six-week-long course titled *Exploring GB1 Protein Dynamics: A Graph Theoretical Perspective*.

**Lecturer, Kadir Has University,** Istanbul, Turkey **2024 (Spring Semester)**

- Molecular Biology and Genetics, project-based education
- Protein Modeling and Simulation, project-based education

**Short-term Visiting Scholar at Pennsylvania State University,** University Park, PA, USA **2024 (January)**

- Collaboration with Dr. Melik C. Demirel
- Predicting the materials properties of tandem repeat proteins.

**Short-term Visiting Scholar at University of Texas Southwestern,** Dallas, TX, USA **2023 (February)**

- Collaboration with Dr. Erdal Toprak
- Drug design and bioinformatics analyses of bacteria drug resistance pathways.

**Virtual Workshop in the MIDST of Centrality and Community Detection in Dynamic Residue Networks** **2021 (March)**

- A full-day workshop as a part of global Biophysical Week (View on Website).

**Teaching Assistant (Virtual), University of Texas Southwestern Medical Center,** Dallas, Texas, USA **2021 (February)**

- Micro course: *Protein Structures as Residue Networks (PSARN)*, five weeks.

**Teaching Assistant, Sabanci University,** Istanbul, Turkey **2015 – 2021**

- Science of Nature (NS 101), seven semesters.
- Introduction to Bioinformatics (BIO 310), two semesters.
- Computational Biology (ENS 210), one semester.
- Computational Approaches to Problem Solving (IF 100), one semester.
- Fundamentals of Nanoscience (NS 218), one semester.
- Computational Techniques for Materials at the Nano-scale (MAT 306), one semester.
- Graduation Project (ENS 491 – 492), Co-supervisor with Dr. Canan Atilgan.
  Project Title: *Carving Lattices to Construct Protein-Like Structures*.

**Short-term Visiting Researcher, Rhodes University,** Grahamstown, South Africa **2017 (August)**

- Collaboration with Dr. Özlem Taştan Bishop
- Project Title: *Scanning Resistance Conferring Mutants of DHFR to Specify Drugs Optimizing Inhibition.*

## SKILLS

**Languages**: English (Proficient, YDS: 85)
**Programming:** Python (Advanced) – scipy, numpy, scikit-learn, matplotlib, networkx; Tcl (Advanced); advanced knowledge of Linux distributions; Bash scripting (Intermediate); MATLAB (Intermediate); Julia (Basic); R (Basic).

## PAPERS

- Guclu, T.F., Tayhan, B., Cetin, E., Atilgan, A.R. and Atilgan, C., **High Throughput Mutational Scanning of a Protein via Alchemistry on a High-Performance Computing Resource.** *Concurrency and Computation: Practice and Experience*, 2025, 37, e8371. https://doi.org/10.1002/cpe.8371 – Research Article (Published). **(Corresponding Author)**

- Guclu T.F., Atilgan A.R., Atilgan C., **Deciphering GB1's Single Mutational Landscape: Insights from MuMi Analysis**. *The Journal of Physical Chemistry B*, 2024, 128 (33), 7987-7996. https://doi.org/10.1021/acs.jpcb.4c04916 – Research Article (Published). **(Corresponding Author)**
- Guclu T.F., Atilgan A.R., Atilgan C., **Dynamic Community Composition Unravels Allosteric Communication in PDZ3**. *The Journal of Physical Chemistry B*, 2021, 125 (9), 2266-2276. https://doi.org/10.1021/acs.jpcb.0c11604 – Research Article (Published).
- Kantarcioglu I., Gaszek I.K., Guclu T.F., Yildiz M.S., Atilgan A.R., Toprak E., Atilgan C., **Structural shifts in TolC facilitate Efflux-Mediated *β*-lactam resistance**. *Communications Biology*, 2024, 7, 1051. https://doi.org/10.1038/s42003-024-06750-0 – Research Article (Published).
- Cetin E., Guclu T.F., Kantarcioglu I., Gaszek I.K., Toprak E., Atilgan A.R., Dedeoglu B., Atilgan C., **Kinetic Barrier to Enzyme Inhibition Is Manipulated by Dynamical Local Interactions in *E. coli* DHFR**. *Journal of Chemical Information and Modeling*, 2023, 63 (15), 4839-4849. https://doi.org/10.1021/acs.jcim.3c00818 – Research Article (Published).
- Guclu T.F., Kocatug N., Atilgan A.R., Atilgan C., **N-Terminus of the Third PDZ Domain of PSD-95 Orchestrates Allosteric Communication for Selective Ligand Binding**. *Journal of Chemical Information and Modeling*, 2021, 61 (1), 347-357. https://doi.org/10.1021/acs.jcim.0c01079 – Research Article (Published).

## CURRENT PROJECTS

- Mutational analysis of dihydrofolate reductase using free energy perturbation simulations to explain antibiotic resistance *en masse*, pilot access applications for MareNostrum 5 Supercomputer (640,000 node hours approximately 80,000 EUR worth) – role: PI; researchers: Dr. Ali Rana Atilgan and Dr. Canan Atilgan **2024 – present**
- Predicting the materials properties of tandem repeat proteins – in collaboration with Dr. Melik C. Demirel **2024 – present**
- High throughput mutational scanning of dihydrofolate reductase via in-silico alchemistry – in collaboration with Dr. Erdal Toprak, Dr. Ali Rana Atilgan and Dr. Canan Atilgan **2023 – present**

## TUBITAK PROJECTS

- "Fonksiyonel Proteinlerin Dinamik Konformasyon Uzaylarında Tam Navigasyon Sağlayan Bütünleştirici Hesaplama Modeli", 122F149, 1001 - Araştırma – *Postdoctoral scholarship* **2024 – 2025**
- "Beyne İlaç Taşımak İçin Beyin Kılcal Damarlarında Bulunan Transitoz Proteinlerinin Hesaplamalı ve Deneysel Yöntemlerle Belirlenmesi", 122S347, 1001 - Araştırma – *Researcher* **2022 – 2025**
- "Supramoleküler Simetri Gösteren Nanoskopik Yapıların Sınıflandırılması", 117F389, 1001 - Araştırma – *PhD student scholarship* **2018 – 2021**
- "Katlanmış Proteinlerin Serbest Enerji Yüzeylerinin "Hesaplamalı Kuvvet Mikroskopisi" Ile Haritalanması", 116F229, 1001 - Araştırma – *PhD student scholarship* **2017 – 2018**
- "Hücre İçinde Demir Taşıyan Proteinlerde Demir Bağlama-Bırakma Dinamiğinin Hesaplamalı ve Deneysel Yöntemlerle İncelenmesi", 113Z408, Uluslararası – *PhD student scholarship* **2015 – 2016**

## PRESENTATIONS

- Guclu T.F., Atilgan C., Atilgan A.R. Hydrogen bond networks reveal key residues in DHFR function, 24th International Symposium on "Disordered Systems: Theory and Its Applications" (DSS-2024), 21–23 November 2024. – Contributed Talk
- Guclu T.F., Atilgan A.R., Atilgan C. A simple mutation-minimization scheme elucidates the fitness landscape of GB1 binding to IgG-Fc, BPS 2024, 68th Biophysical Society Annual Meeting, Philadelphia, Pennsylvania, USA, February 2024. DOI: https://doi.org/10.1016/j.bpj.2023.11.291. – Panel Talk
- Guclu T.F. EuroHPC experience presentation: View on Youtube
- Guclu T.F., Kocatug N., Atilgan C., Atilgan A.R. Allosteric Communication in PDZ3 is Orchestrated by the Charged N-Terminus, BPS 2021, 65th Biophysical Society Annual Meeting, Virtual, USA, February 2021. – Panel Talk
- Guclu T.F., Atilgan C., Atilgan A.R. Ligand Switching Mutations in PDZ Domain Explained by Centrality of Amino Acids, HIBIT 2020, Virtual, Istanbul, Turkey, October 2020. – Selected Talk
- Guclu T.F., Kocatug N., Atilgan C. Protein Dynamics and Function in Solution: Ligand Preferences of a Model Protein Explained by Flexible Region Conformations and Binding Site Interactions, 23rd Liquid State Symposium, Istanbul, Turkey, December 2019. – Contributed Talk
- Guclu T.F., Kocatug N., Atilgan C. Point Mutations Leading to Ligand Switching in PDZ Domains Explained by a Simple Network Analysis, EEBST 2019 – Ecology and Evolutionary Biology Symposium, Ankara, Turkey, July 2019. – Poster Presentation
- Guclu T.F., Kocatug N., Atilgan C. Point Mutations That Lead Induced Ligand Switching in PDZ Domains Are Investigated with Network Analysis, 12th Chemical Physics Congress, Safranbolu, Turkey, October 2018. – Poster Presentation (Poster Award) and Flash Talk
- Guclu T.F., Kocatug N., Atilgan A.R., Atilgan C. A Network Theory Approach to Investigate Point Mutation Induced Ligand Switching in PDZ Domains, 25th Statistical Physics Days, Izmir, Turkey, June 2018. – Short Talk
- Guclu T.F., Musyoka T.M., Tamer Y.T., Toprak E., Atilgan A.R., Tastan Bishop Ö., Atilgan C. Scanning Resistance Conferring Mutants of DHFR to Specify Drugs Optimizing Inhibition, 5th International BAU Drug Design Congress, Istanbul, Turkey, October 2017. – Poster Presentation
- Guclu T.F., Atilgan A.R., Atilgan C. Mutations Affecting Centrality of Residues Confer Antibiotic Resistance in DHFR, 24th Statistical Physics Days, Izmir, Turkey, June 2017. – Short Talk
- Guclu T.F., Atilgan A.R., Atilgan C. Centrality of Residues and Redundancies in Their Communication Explain the Disruptive Mutations in DHFR, From Computational Biophysics to Systems Biology Workshop 2016 (CBSB16), Ankara, Turkey, May 2016. – Contributed Talk
- Guclu T.F., Atilgan A.R., Atilgan C. Disruptive Mutations Elucidated by Centrality of Residues and Redundancies in Inter-Residue Communication Pathways, 41st Federation of European Biochemical Societies (FEBS) Congress, Kuşadası, Turkey, September 2016. – Contributed Talk (Cancelled, Abstract Published)
- Guclu T.F., Atilgan A.R., Atilgan C. Centrality and Path Length of Residues, and Alterations in Their Communication Network Explain the Mutations in DHFR, 23rd Statistical Physics Days, Istanbul, Turkey, June 2016. – Short Talk

## PEER REVIEW ACTIVITIES

- Reviewer for *ACS Omega*
- Reviewer for *Biochemistry and Biophysics Reports*
- Reviewer for *Journal of Chemical Information and Modeling*
- Reviewer for *PROTEINS: Structure, Function, and Bioinformatics*

**CODES**

- Jupyter Notebook for Community Analysis (View on GitHub)
- Pipeline Codes for Molecular Dynamics (MD) (View on GitHub) and Free Energy Perturbation (FEP) Simulations (View on GitHub)
- Pipeline Codes for MD trajectory analyses (View on GitHub)
- Sample Codes from MAT306 hands-on sessions (View on GitHub)
- Pipeline Codes for Mass FEP simulations (View on GitHub)
- Pipeline Codes for Mutation and Minimization (MuMi) scheme (View on Github)

**TRAINING**

- Bilkent University Machine Learning Summer School **2020**
- Koç University Machine Learning Summer School **2019**
- Boğaziçi University Machine Learning Summer School **2018**
- Workshop on Quantitative Evolutionary Biology **2016**

**RERERENCES**

- Canan Atilgan – Professor, thesis advisor
  Faculty of Engineering and Natural Sciences
  Sabanci University, Tuzla 34956, Istanbul, Turkey
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- Melik C. Demirel – Professor, colleague in Tandem Repeat project
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- Fyodor Kondrashov – Professor, reference for lecturing at School of Molecular and Theoretical Biology
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- Özge Şensoy – Associate professor, progress/PhD thesis jury member, colleague
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