

ARZU UYAR, Ph.D.

Principal Investigator of The UBioModel Group - Uyar Lab at IZTECH

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RESEARCH INTERESTS

Molecular dynamics (MD) and enhanced sampling (ES) simulations • Machine learning • Hybrid method development using MD and ES simulations, Elastic Network Modeling and Monte-Carlo algorithm • Virtual screening and docking • Virus-receptor, protein-ligand (drug), protein-nucleic acid interactions • Antibody/nanobody-antigen interactions • Allosteric regulation

EDUCATION

Bogazici University (Istanbul, Turkey)	
Ph.D. Chemical Engineering	06/2014
M.Sc. Chemical Engineering	01/2008
Istanbul University (Istanbul, Turkey)	
B.Sc. Chemical Engineering	06/2004

RESEARCH EXPERIENCE

ASSISTANT PROFESSOR	04/2022-present
Izmir Institute of Technology (IZTECH)	
1. Department of Bioengineering	
2. Computational Science and Engineering Graduate Program	
POSTDOCTORAL RESEARCHER	06/2016-06/2021
Michigan State University (Michigan, US), 5-year J-1 Scholar Program	
Advisor: Dr. Alex Dickson,	
Department of Biochemistry and Molecular Biology	
VISITING RESEARCHER	01/2016-06/2016
Bogazici University (Istanbul, Turkey)	
Advisor: Dr. Pemra Doruker, Polymer Research Center.	
Department of Chemical Engineering	

POSTDOCTORAL RESEARCHER 12/2014-12/2015
Karolinska Institutet (Stockholm, Sweden)
Advisor: Dr. Lennart Nilsson, Department of Biosciences and Nutrition

VISITING RESEARCHER 07/2014-12/2014
Bogazici University (BOUN) and Kadir Has University (Istanbul, Turkey)
Advisors: Dr. Pemra Doruker, Polymer Research Center.
Department of Chemical Engineering, BOUN
Dr. Demet Akten Akdogan, Department of Bioinformatics
and Genetics, Kadir Has University

GRADUATE STUDENT 02/2008-06/2014
Bogazici University (Istanbul, Turkey)
Advisor: Dr. Pemra Doruker
Ph.D. Thesis: “Conformational Transitions of Proteins Using
Multi-Scale Modeling Approaches”

MASTER STUDENT 09/2005-01/2008
Bogazici University (Istanbul, Turkey)
Advisor: Dr. Pemra Doruker
M.Sc. Thesis: “Structure – Function Relationships of Type II Restriction Endonucleases”

UNDERGRADUTE RESEARCH ASSISTANT 2003 - 2004
Istanbul University (Istanbul, Turkey)
Advisor: Dr. Gulin Selda Pozan, Process and Reactor Design,
Department of Chemical Engineering
Poster Title: “Catalytic hydrodechlorination of 2,4-dichlorophenol on
Pd/Rh/C Catalysts”, The International Chemical Engineering Conference
in Paris, France, 2004 (*helped performing experiments in this project*)

UNDERGRADUTE RESEARCH ASSISTANT 2001 - 2003
Istanbul University (Istanbul, Turkey)
Advisor: Dr. Betul Arıkan, Physical Chemistry, Department of Chemistry
*Setting up experiments, performing initial tests in the physical chemistry lab
at the beginning of each semester and grading undergraduate lab reports.*

TEACHING EXPERIENCE

Instructor – Izmir Institute of Technology (IZTECH-Izmir, Turkey) 2022-present
BE584 Molecular Dynamics Methods
BE585 Machine Learning for Computational Biochemistry
BE418 Bioinformatics Tools for Macromolecular Systems
BE417 Macromolecular Dynamics: From Structure to Function
BE305 Statistical Tools for Bioengineers
BE301 Transport Phenomena in Biological Systems

Teaching Assistant – Michigan State University (Michigan, US) 2018-2019
BMB 401 (Online): "Comprehensive Biochemistry" within the scope of the **Postdoc Teaching Internship Program (PTIP)**, ~ **485 students**
Advisor: Dr. Kathleen Foley
Co-Directors: Dr. Kristin Parent and Dr. Jon Kaguni

Project Teaching Assistant (honorary) – Bogazici University (Istanbul, Turkey) 2010
ChE 412 Structure, Function and Simulation of Biopolymers
Advisor: Dr. Pemra Doruker
Mentored 5 groups (**2-3 students in each group**) and
All projects were presented as posters in an international conference - *IX. Chemical Physics Congress*, October 14-16, 2010, Izmir, Turkey.
Poster titles are listed below:

1. "Coupling between Loop Closure and Global Dynamics in Enzymes"
2. "Database of Conformational Transitions with Anisotropic Network Model – Monte-Carlo Methodology"
3. "Conformational Transition Pathway of Adenylate Kinase Using Monte-Carlo Simulations with Collective Moves"
4. "Exploring the Intrinsic Dynamics of Human Beta-2 Adrenergic Receptor and Its Potential Use in Computational Drug Design Studies"

Advised students at IZTECH (*Alphabetically ordered according to last names*)

Main advisor

- Tutku Arslan (Master student)
- Mehmet Emin Aygen (Master student)
- Sefika Baydur (Master student)
- Hatice Tugba Bayer (Master student)
- Hakan Buyuktuncay (Master student)
- Mehmet Can (PhD student)
- Göktürk Cinel (PhD student)
- Ceren Elmaci (Master student)
- Beylem Girgin (Master student)
- Gizem Gokoglu (Master student)
- Sude Gunes (Master student)
- Nursah Halisdemir (Master student)
- Elif Sultan Koc (Master student)
- Ahmet Yigit Savru (Master student)
- Ece Topçu (Master student)

Co-advisor

- Ekin Kestevur-Dogru (PhD Candidate)
- Rukiye Sanli (PhD Candidate)
- Yawer Abbas (Master student)
- Nihat Tolga Filoglu (Master student)
- Fulden Ulucan-Karnak (Master student)

Current Undergraduate Research Project Students: 20 volunteer students - IZTECH

One-to-one Mentoring

Michigan State University (Michigan, US)	2017-2021
Topics: “How to perform and analyze MD simulations, virtual screening and docking”	
Students: 2 undergraduate and 3 graduate students (Alex Dickson Lab)	
1 undergraduate student (Edmund Ellsworth Lab)	
1 undergraduate student (Summer Research Program- ACRES)	
Bogazici University (Istanbul, Turkey)	2006-2016
Topics: “Dynamics of Biomolecular Systems”	
Students: 15 undergraduate and 13 graduate students	
Private instructor (Istanbul, Turkey)	2004-2008
Topics: “Math, science, English language, physics, chemistry, biology, How to read and write in Turkish language”	
Students: >15 (elementary, middle and high school students)	
Online mentoring - epiSTEM Organization (Turkey)	since 2018
Topics: “How to write a scientific project proposal, how to present a scientific work, how to collaborate, coding using Python, performing MD simulations, data analysis using machine learning, and ENM calculations”	
Students: 7 high school students	

PUBLICATIONS

1. Gunes, S; I Arkca; S B Atik; F Ulucan-Karnak; H Taskent Sezgin* and **A Uyar***, “Computational Approaches for Antibody-Based Drug Design” Chapter 11 of the Book “Advances in Drug Delivery Systems for Healthcare – From Concept to Clinic” by IOP Sciences, UK (published *January 2024*), *corresponding authors.
2. Kestevur-Dogru, E; G. Guralp; **A Uyar** and N B Surmeli, “Rational Design of Thermophilic CYP119 for Progesterone Hydroxylation by in Silico Mutagenesis and Docking Screening”, *Journal of Molecular Graphics and Modelling*, 2023, 118, 108323.
3. **Uyar, A** and A Dickson, “Perturbation of ACE2 structural ensembles by SARS-CoV-2 spike protein binding”, *Journal of Chemical Theory and Computation*, **2021**, 17, 9, 5896–5906. (MSU iCER Covid-19 Research Highlights interview video of the study is also available in the link: <https://www.youtube.com/watch?v=XqYMzdOZDis>)
4. Jayaraman S T; J T Kocot; S H Esfahani; N J Wangler; **A Uyar**; Y Mechref; P C Trippier; T J Abbruscato; A Dickson; H Aihara; D A Ostrov and V T Karamyan, “Identification and characterization of two structurally related dipeptides that enhance catalytic efficiency of neurolysin”, *Journal of Pharmacology and Experimental Therapeutics*, **2021**, 379 (2) 191-202; JPET-AR-2021-000840; DOI: <https://doi.org/10.1124/jpet.121.000840>.)
5. Dixon, T; **A Uyar**; S Ferguson-Miller and A Dickson, “Membrane-Mediated Ligand Unbinding of the PK-11195 Ligand from TSPO”, *Biophysical Journal*, **2021**, 120 (1), pp 158-167.
6. Zeng, X*; **A Uyar, ***; D Sui*; N Donyapour; D Wu; A Dickson and J Hu, “Structural Insights into Lethal Contractural Syndrome Type 3 (LCCS3) Caused by a Missense Mutation of PIP5K γ ”, *Biochemical Journal*, BCJ20180326, **2018**. (*equal contribution)
7. **Uyar A.**, V T Karamyan and A Dickson, “Long-range changes in neurolysin dynamics upon inhibitor binding”, *J. Chem. Theory Comput.*, **2018**, 14 (1), pp 444–452.
8. Hartono Y. D., Y. V Pabon, **A Uyar**, J Wengel, K E Lundin, R Zain, C I E Smith, L Nilsson and A Villa, “Role of pseudocytidine tautomerization in triplex forming oligonucleotides: in silico and in vitro studies”, *ACS Omega*, **2017**, 2 (5), pp 2165–2177.
9. Can M.T., Z Kurkcuoglu, G Ezeroglu, **A Uyar**, O Kurkcuoglu and P Doruker, “Conformational Dynamics of Bacterial Trigger Factor in Apo and Ribosome-bound States” *PLOS One*, **2017**, 12(4): e0176262.
10. **Uyar A.**, N Kantarci-Carsibasi, T Haliloglu and P Doruker, “Features of Large Hinge-Bending Conformational Transitions. Prediction of Closed Structure from Open State”, *Biophysical Journal*, **2014**, 106 (12), 2656-2666.
11. Mericer C., D Findik, **A Uyar**, T Haliloglu and P Doruker, “Unbiased and Targeted

Conformational Transition Pathways of Hinge-bending Proteins”, 10th International Conference on Cellular and Molecular Biology, Biophysics and Bioengineering (**BIO14**), **2014**, Istanbul, Turkey. (*This publication includes the results obtained from our hybrid methodology that incorporates weighted-ensemble and Elastic Network Modeling.*)

12. Ozcan O.*, **A Uyar***, P Doruker and E D Akten, “Effect of intracellular loop 3 on intrinsic dynamics of human beta2-adrenergic receptor”, ***BMC Structural Biology***, **2013**, 13 (29) (*selected as **Hot Topic** in *BMC Structural Biology**), **equal contribution.*
13. **Uyar A.**, O Kurkcuoglu, L Nilsson and P Doruker, “The elastic network model reveals a consistent picture on intrinsic functional dynamics of type II restriction endonucleases”, ***Physical Biology***, **2011**, 8 (5), 056001.

FUNDED PROJECTS

1. TUBITAK 1001: 123Z537 – “Identification of Ligand Binding Sites in Biomolecular Systems with Computational and Experimental Approaches”, **PI of the Project**, expected final date: November 2026
2. AUDP-2022-İYTE-3-0041–“Computational and Experimental Methods for Allosteric Binding in Biological Systems”, **PI of the project**, expected final date: January 2026
3. TUSEB A-34359 – **Advisor**, expected final date: June 2024
4. AÜDP-2022-IYTE-2-0060 – **Researcher**, expected final date: August 2024
5. TUBITAK ARDEB-1001: 124S204 – **Researcher**, expected final date: May 2026
6. TUSEB -A-27642 – **Researcher**, expected final date: December 2025

CONFERENCES AND LECTURES

Oral Presentations (English):

1. 5th International / 34th National Biophysics Congress 2023, “Prediction of Allosteric Sites in Multimeric Proteins using a Fast Computational Method ESSA”.
2. American Chemical Society (ACS) Fall 2021, “Learning the differences between apo- and SARS-CoV-2-bound ACE2 structures” (*invited speaker*).
3. Graduate Women in Science (GWIS) Research Triangle Inter/National Seminars, April 2021, “Preventing SARS-CoV-2 Spike Protein Binding by Modulating the ACE2 Conformational Landscape” (*invited speaker*).
4. D. E. Shaw Research Company, “Graduate and Postdoc Women’s Forum”, June 2017, “Exploration of allosteric modulation in neurolysin upon ligand binding using molecular dynamics and machine learning” (*invited speaker*).
5. MWTCC 2017, Michigan State University, “Exploration of allosteric behavior in neurolysin upon inhibitor binding using multiscale computational methods”.
6. Midwest Protein Folding Conference, University of Notre-Dame, 2017, “Dynamical and structural differences in apo and inhibitor-bound neurolysin revealed by molecular dynamics and machine learning”.
7. International Scholar Showcase, Michigan State University (MSU), 2017, “Exploration of Neurolysin Dynamics by Multiscale Computational Approaches” (*MSU International J-1 Scholar of the Month awardee talk*).
8. Annual Meeting of the Swedish Chemical Society Theoretical Chemistry Section 2015- Baltic Lights, Kalmar, Sweden, “Effect of pseudoisocytidine mutation on DNA base upon binding of triplex-forming oligonucleotide”.
9. Membrane Bound Protein & Ligand Docking Workshop, Sabanci University, Tuzla, Turkey 2012, “Effect of Intracellular Loop ICL3 on the Dynamics and Ligand Interactions of Human β 2-Adrenergic Receptor (β 2-AR)”.

Oral Presentations (Native language):

1. Gebze Technical University, Department of Bioengineering, Departmental Seminar Series, 2022. (*invited speaker*)
2. Ege University, Department of Bioengineering, Departmental Seminar Series, 2022. (*invited speaker*)

Poster Presentations:

1. TBS International Biochemistry Congress 2022 – 33rd National Biochemistry Congress, October 2022, “In silico identification of potent modulators that may bind to certain pancreatic adenocarcinoma-associated proteins”.
2. Biophysical Society (BPS) Virtual Networking Event- Biomolecular Modeling in the Age of Machine Learning, May 2021, “Learning the differences between apo- and SARS-CoV-2-bound ACE2 structures”.
3. ACS Spring 2021, “Learning the differences between apo- and SARS-CoV-2-bound ACE2 structures”.
4. Department of Biochemistry and Molecular Biology Retreat, MSU, 2019, “Enhanced Sampling Simulations of Protein Dynamics Using a Novel Weighted Ensemble Algorithm Driven by Collective Variables”.
5. Cisplatin Celebration & Cancer Research Symposium, MSU, 2018, “Disruption of Inter-residue Interaction Network in Pip5ky by a Disease-related Single Mutation Near The Binding Site”.
6. Midwest Protein Folding Conference, University of Notre-Dame, 2018, “Disruption of Inter-residue Interaction Network in Pip5ky by a Disease-related Single Mutation Near The Binding Site”.
7. D. E. Shaw Research Graduate and Postdoc Women’s Forum, June 2017, “Exploration of allosteric modulation in neurolysin upon ligand binding using molecular dynamics and machine learning”.
8. Biophysical Society Meeting, New Orleans, USA, February 2017, “How Does a Ligand Explore the Deep Channel of Neurolysin? A Conformational Dynamics Study with WExplore and Elastic Network Modeling”.
9. Annual Meeting of the Swedish Chemical Society Theoretical Chemistry Section 2015- Baltic Lights, Kalmar, Sweden, “The conformational effect of the binding oligonucleotide on the stability of DNA triplex”.
10. 10th European Biophysics Congress, EBSA, 2015, “Dynamical Features of NF- κ B via Molecular Dynamics Simulations and Elastic Network Models”.
11. Modeling of Biomolecular Systems Interactions, Dynamics, and Allostery Meeting, Istanbul, 2014, “Generation of conformational transition pathways and the prediction of closed structures for proteins”.
12. Biophysical Society Meeting, San Francisco, USA, February 2014, “Assessing Dynamic Features of NF- κ B via Molecular Dynamics Simulations and Elastic Network Model”.

13. Biophysical Society Meeting, San Francisco, USA, February 2014, “Effect of Intracellular Loop 3 on Intrinsic Dynamics of Human β 2-Adrenergic Receptor”.
14. eSSENCE International Workshop on Macromolecular Structure and Dynamics, Uppsala University, Sweden, 2013, “Scissor-like and tong-like motions of NF- κ B (p50) Homodimer from Molecular Dynamics and Anisotropic Network Model Simulations”.
15. X. Chemical Physics Congress, TOBB Economics and Technology University, Ankara, Turkey, October 10-12, 2012, “Conformational Transitions of Proteins using Hybrid Methodologies”.
16. Dynamics of Protein Nucleic Acid Interactions: Integrating Simulations with Experiments workshop by CECAM, Zurich, Switzerland, September 13-16, 2011, “Molecular dynamics and anisotropic network model simulations of a NF-kappaB (p50) homodimer free and in complex with DNA”.
17. IX European Symposium of Protein Society “Wonders and Disasters of the Protein World” Stockholm, Sweden, May 22-26, 2011 “Prediction of protein conformational transitions by the anisotropic network model coupled with Monte Carlo simulations”.
18. ECCB '08 Conference, Sardinia, Italy, September 22-26, 2008, “Elastic network modeling of type II restriction endonucleases complexed with cognate and non-cognate DNA”.
19. FEBS, Istanbul, Turkey, 2006, “Structure-Function Relationship of Restriction Endonucleases”.
20. NDCOS “Workshop on New Directions in Complex Systems”, Istanbul, Turkey, 2006 “Functional dynamics in type II restriction endonucleases”.
21. PROTEOMICS: Workshop on Protein Structure and Function, Antalya, Turkey 2006, “Vibrational Dynamics of the Catalytic Residues in Triosephosphate Isomerase”.

AWARDS AND FELLOWSHIPS

- Researcher fellowship: National Institutes of Health (R01GM130794) 2019-2021
- Earned GPU computing clusters, which are dedicated to the accepted COVID-19 project proposals, iCER MSU 2020
- “J-1 Scholar of the Month” Award, MSU 2017
- EMBO Short-term Fellowship 2013
- ESF Short-term Fellowship 2009
- Graduate student and/or researcher fellowship: TUBITAK 104M247, 109M213, 109M281 and 113M237, Bogazici University 2005-2011
- Graduate student fellowship, BAP 5714P, 7621D, Bogazici University 2012-2014

SELECTED ACADEMIC DISTINCTIONS AND OTHER MERITS

Organization and Committee Membership

- IZTECH Promotion and Public Relations Committee Member since 2022
- Department of Bioengineering MÜDEK Committee Member since 2023
- Co-chair of the Professional Events Committee 2019-2021
National Graduate Women in Science
Annual Meeting 2021, June 10-12
- Cryo-EM faculty search committee Postdoc representative 2017-2019
Department of Biochemistry and Molecular Biology
Michigan State University
- President of Graduate Women in Science Mid-Michigan Chapter 2018-2019
- Co-chair of the Community Outreach Committee in Graduate Women 2017-2019
in Science (GWIS) Mid-Michigan Chapter
- Fellowship Committee member in National Graduate Women in Science 2017-2018
- Media Committee member in National Graduate Women in Science since 2017
- Member of American Chemical Society (ACS) since 2020
- Member of AAAS/Science (nominated by Dr. Erich Grotewold, 2019-2020)
Chair of the Department of Biochemistry and Molecular Biology, MSU) since 2019
- Member of National Postdoc Association, USA since 2019
- General Coordinator II (2018-2020), online mentor, author, editor 2017-2020
and YouTube Live Videos coordinator at epiSTEM, a social project
to transfer scientific developments to the Turkish community via
“Shall We Make an Online Experiment?” and “Coding with Python”
projects, and popular science news
<https://epistemturkiye.org/>

Peer review

- Reviewer for the PeerJ since 2024
- Reviewer for the Turkish Journal of Biology since 2022
- Judge for International Buca IMSEF Art and Science Festival since 2022
- Reviewer for the Journal of Chemical Information and Modeling since 2022
- Reviewer for the Computational Biology and Chemistry since 2022
- Reviewer for the Computational and Structural Biotechnology Journal since 2021
- Judge for Research Triangle Travel Award by National Graduate Women in Science (GWIS) 2019
- Reviewer for the Scientific Reports by Nature Research 2018
- Judge for the National GWIS Organization Fellowships since 2018
- Judge for the Graduate Academic Conference, Michigan State University 2018
- Judge for the University Undergraduate Research&Arts Forum (UURAF) 2018

Science Outreach Activities

- *Invited Speaker*, Buca IMSEF Art and Science Festival, Turkey, 2022
- *Activity Leader / Volunteer Track Leader*,
 - Woldumar Nature Center (WNC) Campfire Science Night, Michigan State University (MSU) Science Festival, 2018 and 2019
 - American Heritage Festival at WNC, 2018
 - Hiawatha Science Festival, Michigan, 2018
 - Darwin Discovery Day, MSU Museum, since 2018
 - Girls Math and Science Day, MSU, 2018
 - Girls' STEM Day, MSU, since 2017
 - Grandparents University, MSU, 2017
- *Invited Speaker*, WNC Summer Camp for high school students, Michigan, 2018

Science Communication Workshops

- “Improv for Scientists to Improve Public Communication Skill” by Alan Alda Center 2017
- “ComSciCon-Michigan”, The communicating science workshop 2018

Personal Skills

Techniques: CHARMM • Openmm • NAMD • PyMOL • VMD • Schrödinger Glide
Schrödinger Maestro • Autodock Vina • Chimera • ProDy

Programming Languages: Python • Fortran • MATLAB • Tcl

Languages: English (advanced) • German (beginner) • Swedish (beginner) • Turkish (native)