

Curriculum Vitae



Name : Ebru Demet Akten
Address : Department of Molecular Biology and Genetics, Faculty of Engineering and Natural Sciences, Kadir Has University, Kadir Has Cad, Cibali 34083, Istanbul, Turkey.
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Citizenship : Turkey
Birth date : July 21st, 1971

EDUCATION

- **Ph.D. in Polymer Science:**
Thesis title: *Computer Simulation of Polyolefins and Monte Carlo Simulation of Rotational Isomeric State (RIS) Chains on a High-Coordination Diamond Lattice*
Ph.D. advisor: Prof. Wayne L. Mattice
Institute of Polymer Science, University of Akron, Akron, OH, Jan 2001
- **M.S. in Chemical Engineering:**
Thesis title: *Simulation of Protein Structure by a Simplified Model: Application to the Rop Dimer*
M.S. advisors: Prof. Ivet Bahar, Prof. Burak Erman
Dept. of Chemical Engineering, Bogazici University, Istanbul, Turkey, May 1996
- **B.S. in Chemical Engineering:**
Dept. of Chemical Engineering, Bogazici University, Istanbul, Turkey, May 1994
- **High school:**
Lycée de Galatasaray, Istanbul, Turkey, June 1990

INDUSTRIAL AND ACADEMIC EXPERIENCE

- **Kadir Has University, Professor (2020 – present):**
Full time faculty member at the Department of Bioinformatics and Genetics.
- **Kadir Has University, Associate Professor (2013 – 2020):**
Full time faculty member at the Department of Bioinformatics and Genetics.
- **Kadir Has University, Assistant Professor (2008 – 2013):**
Full time faculty member at the Department of Information Technologies.
- **Bogazici University, Research Scientist (2008, 8 months):**
Full time researcher at Polymer Research Center.
- **Haliç University, Assistant Professor (2006 – 2008):**
Full time faculty member at the Department of Molecular Biology and Genetics.
- **Genomics Institute of the Novartis Research Foundation (2002 – 2004):**
Postdoctoral scholar under the supervision of Prof. Peter Schultz in the Computational Discovery group.
- **Carnegie Mellon University, (2001 – 2002):**
Postdoctoral scholar in the research group of Prof. David Sholl in the Department of Chemical Engineering.
- **University of Akron, (1996 – 2001):**
Research Assistant in the research group of Prof. Wayne L. Mattice in the Institute of Polymer Science.
- **Bogazici University, (1994 – 1996):**
Research Assistant under the supervision of Prof. Ivet Bahar in Polymer Research Center at Bogazici University, Istanbul, Turkey.

SELECTED SCIENTIFIC SKILLS

- Molecular Dynamics simulation in Molecular Mechanics
- Allosteric communication networks in proteins
- Protein's structure, dynamics and function at the molecular level
- Computer-aided drug design
- Conformational statistics of macromolecules
- Coarse-grained and fully atomistic modeling
- Development of empirical and knowledge-based potentials

TECHNICAL SKILLS

- Unix (Linux, IRIS, BSD-MacOS) operating system, cluster experience
- Unix scripting languages and utilities; csh, tcsh, make
- Source code development in C and Fortran programming languages
- Matlab
- LaTeX typesetting
- Molecular graphics visualization tools; VMD (Visual Molecular Dynamics), PyMOL, MOE
- Commercial packages:
 - NAMD (Nanoscale Molecular Dynamics)
 - Autodock (Automated Docking Tools)
 - GOLD Docking Tool (CCDC)
 - Glide (Schrödinger Inc.)
 - MOE (Molecular Operating Environment)
 - LigandScout / Inteligand
 - MSI BIOSYM/InsightII and MSI Cerius2
- Fluent in both English and French

PUBLICATIONS IN SCI/ SSCI/ AHI JOURNALS

1. Fidan, V.G, Nayir I, Aydin D., **Akten ED**, "Reshaping Globular Dynamics of *S.aureus* Pyruvate Kinase via Bond Restraints to Allosteric Site, J Comput Aided Mol. Design, (2025), 40:6
2. Yüksek, Aslı; Yıkınç, Batuhan; Nayır, İrem; Alnıgeniş, Defne; Fidan, Vahap Gazi; Topuz, Tayyip; **Akten ED**, "Structural Descriptors for Subunit Interface Regions in Homodimers: Effect of Lipid Membrane and Secondary Structure Type", Journal of Chemical Information and Modeling, (2025) Vol.65, No.7, 3117-3126.
3. Alayoubi, Oubadah; Poyraz, Yağmur; Hassan, Gana; Gül, Sümeyye Berfin; Çalhan, Nergiz; Mert Şahin, Naz Mina; Gautam, Megha; Kutlu, Aylin; Özuğur Uysal, Bengü; **Akten ED**; Pekcan, Önder, "Hydrogels from Protein-Polymer Conjugates: A Pathway to Next-Generation Biomaterials", Gels, (2025) Vol.11, No.2.
4. Guner-Yilmaz OZ, Kurkcuoglu O, **Akten ED**, "Tunnel-like region observed as a potential allosteric site in *Staphylococcus aureus* Glyceraldehyde-3-phosphate dehydrogenase", Archives of Biochemistry and Biophysics, Vol:752 (2024)
5. Sogunmez N, **Akten ED**, "Information Transfer in Active States of Human β_2 -Adrenergic Receptor via Inter-Rotameric Motions of Loop Regions", Applied Sciences, Vol:12, 8530, (2022)
6. Celebi M., **Akten ED**, "Altered Dynamics of *S.aureus* Phosphofructokinase via Bond Restraints at Two Distinct Allosteric Sites", Journal of Molecular Biology, Vol:434(7), 167646, (2022).
7. Celebi M., Inan T., Kurkcuoglu O., **Akten ED**, "Potential Allosteric Sites Captured in Glycolytic Enzymes via Residue-Based Network Models: Phosphofructokinase, Glyceraldehyde-3-Phosphate Dehydrogenase and Pyruvate Kinase", Biophysical Chemistry, Vol:280, 106701, (2022)
8. Metin R., **Akten ED**, "Drug Repositioning to Propose Alternative Modulators for Glucocorticoid

Receptor through Structure-Based Virtual Screening", J Biomol Str & Dyn, <https://doi.org/10.1080/07391102.2021.1960608>, (2021)

9. Hu G, Doruker P, Li H, **Akten ED**, "Editorial: Understanding Protein Dynamics, Binding and Allostery for Drug Design", *Frontiers in Molecular Biosciences*, Vol:8, Article 681364 (2021).
10. Sogunmez N, **Akten ED**, "Distinctive Communication Networks in Inactive States of β_2 -Adrenergic Receptor: Mutual Information and Entropy Transfer Analysis", *Proteins: Structure, Function and Bioinformatics*, Vol:88(11), 1458-1471 (2020).
11. Ayyildiz M, Celiker S, Ozhelvacı F, Akten ED, "Identification of Alternative Allosteric Sites in Glycolytic Enzymes for Potential Use as Species-Specific Drug Targets", *Frontiers in Molecular Biosciences*, Vol:7, Article 88 (2020).
12. Sogunmez N, **Akten ED**, "Intrinsic Dynamics and Causality in Correlated Motions Unraveled in Two Distinct Inactive States of Human β_2 -Adrenergic Receptor (β_2 -AR)", *J Physical Chemistry B*, Vol: 123 (17), 3630-3642 (2019)
13. Dilcan G, Doruker P, **Akten ED**, "Ligand-Binding Affinity of Alternative Conformers of Human β_2 -adrenergic Receptor in the Presence of Intracellular Loop 3 (ICL3) and Their Potential Use in Virtual Screening Studies", *Chemical Biology and Drug Design*, Vol: 93 (15), 883-899 (2019)
14. Cifci G, Aviyente V, **Akten ED**, Monard G, "Assessing protein-ligand binding modes with computational tools: the case of PDE4B", *J Comput Aided Mol Des*, Vol: 31(6), 563-575 (2017).
15. Ozgur C, Doruker P, **Akten ED**, "Investigation of Allosteric Coupling in Human β_2 -adrenergic Receptor in the Presence of Intracellular Loop 3", *BMC Struct Biol*, Vol:16, 9 (2016).
16. Ozyigit I, **Akten ED**, Pekcan O, "Structural Analysis of Peptide Fragments Following the Hydrolysis of Bovine Serum Albumin by Trypsin and Chymotrypsin", *J Biomol Str & Dyn*, Vol: 34, pp:1092-1100 (2016)
17. Kurkcuoglu Z, Findik D, **Akten ED**, Doruker P, "How an inhibitor bound to subunit interface alters triosephosphate isomerase dynamics", *Biophysical J*, Vol:109, pp:1169-1178 (2015)
18. Koroglu A, **Akten ED**, "Transmembrane helix 6 observed at the interface of β_2 AR homodimers in blind docking studies", *J Biomol Str & Dyn*, Vol:33, pp:1503-1515 (2015)
19. Yakar R, **Akten ED**, "Discovery of high affinity ligands for beta2 adrenergic receptor through pharmacophore-based high-throughput virtual screening and docking". *J Mol Graph & Model*, Vol: 53, 148-160 (2014)
20. Ozcan O, Uyar A, Doruker P, **Akten ED**, "Effect of intracellular loop 3 on intrinsic dynamics of human beta-2 adrenergic receptor". *BMC Struct Biol*, Vol:13, 29 (2013)
21. Cakan S, **Akdoğan ED**, "Exploring distinct binding site regions of beta-2 adrenergic receptor via coarse-grained molecular dynamics simulations". *Turkish J of Chem*, Vol:35, 449-463 (2013)
22. Cifci G, Aviyente V, **Akten ED**, "Molecular Docking Study Based on Pharmacophore Modeling for Novel Phosphodiesterase IV Inhibitors". *Molecular Informatics*, Vol:31, pp:459-471 (2012)
23. Kurkcuoglu Z., Ural G., **Akten ED**, Doruker P. "Blind Docking of Benzothiazoles to Multiple Receptor Conformations of Triosephosphate Isomerase from *Trypanosoma cruzi* and Human". *Molecular Informatics*, Vol:30, pp:986-995 (2011)
24. **Akdoğan ED**, Erman B, Yelekci Y, "In silico Design of Novel and Highly Selective Lysine-Specific Histone Demethylase Inhibitors". *Turkish J of Chem*, Vol:35, 1-20 (2011)
25. **Akten ED**, Cansu S and Doruker P, "A Docking Study Using Atomistic Conformers Generated via Elastic Network Model for Cyclosporin A/Cyclophilin A Complex". *J Biomol Str & Dyn*, Vol:27, pp:13-25 (2009)
26. **Akten ED**, Siriwardane, R., and Sholl, D., "Monte Carlo Simulation of Single- and Binary-Component Adsorption of CO₂, N₂, and H₂ in Zeolite Na-4A". *Energy and Fuels*, Vol:17, pp:977-983 (2003)
27. Goj A, Sholl D, **Akten ED**, and Kohen D, "Atomistic Simulation of CO₂ and N₂ Adsorption in Silica Zeolites: The Impact of Pore Size and Shape". *J Phys Chem B*, Vol:106, pp:8367-8375 (2002)
28. **Akten ED** and Mattice WL "Monte Carlo Simulation of Head-to-Head, Tail-to-Tail Polypropylene and Its Mixing Behavior with Polyethylene in the Melt". *Macromolecules*, Vol:34, pp:3389-3395 (2001)

BOOK CHAPTER:

- Akten, E. D., Mattice, W. L. and Suter, U. W. "Rotational Isomeric State (RIS) Calculations, with an Illustrative Application to Head-to-Head, Tail-to-Tail Polypropylene" in **Simulation Methods for Modeling Polymers**, Kotelyanskii, M.; Theodorou, D. N., Eds., Marcel Dekker, pp 89-107 (2004)

RESEARCH PROJECTS:

1. **TÜSEB** (39551): "Uncovering potential allosteric sites in glycolytic enzymes of bacterial and parasitic species to be used as target in species-specific drug design". **Project Director**. Budget: 180.000,00 TL (Dec 2024- Dec 2025)
2. **TÜBİTAK-1001** (221Z078). "Structural Fingerprints of Interface Regions in Protein Complexes: Prediction of Interface via Machine Learning Techniques". **Project Director**. Budget: 604.473,00 TL (2022-2025)
3. **TÜBİTAK-1001** (218M320). "Identification of species-specific regions in glycolytic enzymes and their use in allosteric drug design studies". **Project Director**. Budget: 707.756,00 TL (2019-2022)
4. **TÜBİTAK-1002** (119M188) "Factors Affecting the Amino acid Propensity and Interactions in Interior, Surface and Interface Regions of Protein Complexes: Membrane Environment, Secondary Structure and Number of Monomer Units". **Project Director**. Budget: 45.000,00 TL (2019-2020)
5. **TÜBİTAK-1001** (118F412) "Analysis of Finite Metric Spaces via Gromov Products and their Applications to Phylogenetics". **Researcher** (Project Director: Prof. Ayşe Hümeysra Bilge). Budget: 263.500,00 TL (2019-2021)
6. **TÜBİTAK-1001** (213M544). "Investigating the Allosteric Mechanism in β_2 Adrenergic Receptor upon Activation/Inactivation and its Application in Drug Design". **Project Director**. Budget: 257.420,00 TL (2014-2016)
7. **TÜBİTAK-1001** (113M237). "New computational approaches to unravel allosteric mechanisms and ligand binding sites". **Researcher** (Project Director: Prof. Pemra Doruker Turgut). Budget: 238.000,00 TL (2013-2016)
8. **TÜBİTAK-1001** (109M281). "Exploring the Dynamic Structure of β_2 Adrenergic Receptor and its Importance in Computer-Aided Drug Design". **Project Director**. Budget: 181.300,00 TL (2009-2012)
9. **TÜBİTAK-1001** (109M213). "Development and application of hybrid algorithms for studying protein flexibility and conformational transitions". **Researcher** (Project Director: Prof. Pemra Doruker Turgut). Budget: 234.145,00 TL (2009-2012)

SUPERVISED GRADUATE THESIS:

1. "Latife Sude Vural. Master Student at Kadir Has University, "Detection Of Allosteric Sites For Designing Species-Specific Allosteric Inhibitors In Hexokinase And Increasing The Potency Of Inhibition For St2 Receptor" (2023-2025)
2. Metehan Çelebi. Master Student at Kadir Has University, "Allosteric Inhibition of Phosphofruktokinase through constrained MD simulations" (2019-2021)
3. Nuray Sogunmez. PhD Student at Kadir Has University, "Allosteric Communication Network in Human β_2 -Adrenergic Receptor (β_2 -AR)" (2016-2020)
4. Merve Ayyıldız. Master Student at Kadir Has University, "Determination of Novel Allosteric Sites in Glycolytic Enzymes and their Use in Species-Specific Drug Design" (2018-2020)
5. Serkan Çeliker. Master Student at Kadir Has University, "Determination of Novel Allosteric Sites in Glycolytic Enzymes and their Use in Species-Specific Drug Design" (2018-2020)"
6. M. Fatih Özhelvacı. Master's Thesis. Boğaziçi University, Computational Science and Engineering, **co-advisor**. "Determination of Species-Specific Allosteric Binding Sites in Pyruvate Kinase and its Use in Drug Design Studies" (2019-2020)
7. Gonca Dilcan. Master's Thesis. Kadir Has University, Computational Biology and Bioinformatics, **advisor**. "Classification of Distinct Conformers of β_2 -Adrenergic Receptor (β_2 -AR) Based on Binding Affinity of Ligands through Docking Studies" (2015-2017)
8. Canan Özgür. Master's Thesis. Boğaziçi University, Computational Science and Engineering, **co-advisor**. "Allosteric Mechanism in Human β_2 -Adrenergic Receptor". (2012- 2014)
9. Ayça Koroğlu. Master's Thesis. Kadir Has University, Computational Biology and Bioinformatics, **advisor**. "Prediction of 3D structure of the Dimeric State of Human β_2 -Adrenergic

- Receptor*". (2010-2016)
10. Rüya Yakar. Master's Thesis. Kadir Has University, Computational Biology and Bioinformatics, advisor. "*Pharmacophore Screening and Docking Studies to Explore Novel Inhibitors for Human β -Adrenergic Receptor*". (2010-2013)
 11. Sibel Çakan. Master's Thesis. Kadir Has University, Computational Biology and Bioinformatics, advisor. "*Exploring Intrinsic Dynamics of Human B2-Adrenergic Receptor through Coarse-Grained Molecular Dynamics*". (2010-2012)
 12. Özer Özcan. Master's Thesis. Boğaziçi University, Computational Science and Engineering, co-advisor. "*Structural Dynamics of Human B2-Adrenergic Receptor*". (2010-2011)

COURSES TAUGHT:

- **Courses thought at Kadir Has University:**
 - Undergraduate courses:
 - Molecular Modeling and Simulation
 - Bioinformatics I & II
 - Computer-Aided Drug Design
 - Structured Programming (C programming language)
 - Numerical Methods and Optimization (Application with Matlab)
 - Introduction to Operating Systems
 - Computational Structural Biology
 - Introduction to Bioinformatics
 - Graduate courses:
 - Bioinformatics I & II
 - Computer-Aided Drug Design
 - Molecular Modeling and Graphics
 - Molecular Modeling, Simulation and Visualization Techniques
 - Proteins in Action