

Assoc. Prof. Mert Gür

Personal Information

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International Researcher IDs

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Biography

Dr. Gur earned his PhD degree in Computational Science and Engineering at Koç University in 2010 and his Bachelor's degree from the Department of Mechanical Engineering at Middle East Technical University in 2006. Following his graduation, he was awarded the position of a postdoctoral associate in the Department of Computational and Systems Biology at the University of Pittsburgh's School of Medicine. During this time, he became jointly appointed as a Lecturer in the Department of Mechanical Engineering and Material Science, at University of Pittsburgh. In 2014 he joined the Joint Center for Artificial Photosynthesis at Lawrence Berkeley National Laboratory as a postdoctoral fellow. In 2015 Dr. Gur was appointed as a Faculty member at the rank of assistant professor in the in the Department of Mechanical Engineering at Istanbul Technical University. He worked as a visiting scholar in the Department of Computational and Systems Biology at the University of Pittsburgh during the summer 2016 and in the Chemistry Department at University of California, Berkeley throughout summer 2017. Dr. Mert Gur received the Turkish Academy of Sciences (TÜBA) Outstanding Young Scientists Award (GEBİP) in 2016. His research interests are in the areas of (i) Biomolecular machines, motors, and systems (ii) Computational simulation and modeling, (iii) Drug Design, and (iv) Food Drying. He joined the editorial board of Journal of Molecular Graphics and Modelling in 2016.

Education Information

Doctorate, Koc University, Institute Of Science, Turkey 2007 - 2010

Undergraduate, Middle East Technical University, Faculty Of Engineering, Makine Mühendisliği Bölümü, Turkey 2000 - 2006

Foreign Languages

German

English

Dissertations

Doctorate, Binding and mode coupling of proteins, Koç Üniversitesi, Fen Bilimleri Enstitüsü, 2010

Research Areas

Health Sciences, Medicine, Fundamental Medical Sciences, Biostatistics and Medical Informatics, Biochemistry, Technical Sciences, Mechanical Engineering, Thermodynamics, Basic Sciences, Life Sciences, Biophysics, Molecular Biophysics, Molecular Biology and Genetics, Protein Engineering

Academic Titles / Tasks

Associate Professor, Istanbul Technical University, Makina, Makina Mühendisliği, 2021 - Continues
Assistant Professor, Istanbul Technical University, Makina, Makina Mühendisliği, 2018 - 2021
Assistant Professor, Istanbul Technical University, Makina, Makina Mühendisliği, 2015 - 2018
Assistant Professor, University of California, Berkeley, Kimya, Kimya, 2017 - 2017
Assistant Professor, University of Pittsburgh, Tıp Fakültesi, Hesaplamalı Biyoloji Ve Sistem Biyolojisi, 2016 - 2016
Research Assistant, University of Pittsburgh, Tıp Fakültesi/School Of Medicine, Hesaplamalı Biyoloji Ve Sistem Biyolojisi Bölümü/Department Of Computational And Systems Biology , 2010 - 2014
Lecturer PhD, University of Pittsburgh, Mühendislik Fakültesi/Swanson School Of Engineering, Makina Mühendisliği Ve Malzeme Bilimi Bölümü/Department Of Mechanical Engineering And Material Science, 2012 - 2012
Research Assistant, Koc University, Institute Of Science, Hesaplamalı Bilimler Ve Mühendislik (Dr), 2007 - 2010
Research Assistant, Koc University, Institute Of Science, Makine Mühendisliği (Yl) (Tezli), 2006 - 2007

Academic and Administrative Experience

Vice Dean, Istanbul Technical University, Makina, Makina Mühendisliği, 2020 - Continues
Assistant Director of the Institute, Istanbul Technical University, Fen Bilimleri Enstitüsü, 2018 - 2020

Courses

MAK 370 - Uygulamalı Isı Geçişi, Undergraduate, 2016 - 2017

Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Binding Mechanism of Neutralizing Nanobodies Targeting SARS-CoV-2 Spike Glycoprotein**
Golcuk M., Haciosuleyman A., Erman B., Yildiz A., Gür M.
JOURNAL OF CHEMICAL INFORMATION AND MODELING, vol.61, no.10, pp.5152-5160, 2021 (SCI-Expanded)
- II. **Critical Interactions Between the SARS-CoV-2 Spike Glycoprotein and the Human ACE2 Receptor**
Taka E., Yilmaz S. Z., Golcuk M., Kilinc C., Aktas U., Yildiz A., Gür M.
JOURNAL OF PHYSICAL CHEMISTRY B, vol.125, no.21, pp.5537-5548, 2021 (SCI-Expanded)
- III. **THE FIRST LAW OF THERMODYNAMICS ANALYSIS OF TRANSPORTERS INVOLVED IN THE GLUTAMATE/GABA-GLUTAMINE CYCLE**
Gür M., Yilmaz S. Z., Taka E.
ISI BILIMI VE TEKNIGI DERGISI-JOURNAL OF THERMAL SCIENCE AND TECHNOLOGY, vol.41, no.2, pp.265-276, 2021 (SCI-Expanded)
- IV. **Conformational transition of SARS-CoV-2 spike glycoprotein between its closed and open states**
Gür M., Taka E., Yilmaz S. Z., Kilinc C., Aktas U., Golcuk M.
JOURNAL OF CHEMICAL PHYSICS, vol.153, no.7, 2020 (SCI-Expanded)
- V. **Molecular dynamics simulations provide molecular insights into the role of HLA-B51 in Behcet's disease pathogenesis**
Gür M., Golcuk M., Gül A., Erman B.

CHEMICAL BIOLOGY & DRUG DESIGN, vol.96, no.1, pp.644-658, 2020 (SCI-Expanded)

- VI. **Thermodynamic first law efficiency of membrane proteins**
Gür M., Golcuk M., Yilmaz S. Z., Taka E.
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.38, no.2, pp.439-449, 2020 (SCI-Expanded)
- VII. **A novel small-molecule antagonizes PRMT5-mediated KLF4 methylation for targeted therapy**
Zhou Z., Feng Z., Hu D., Yang P., Gur M., Bahar I., Cristofanilli M., Gradishar W. J., Xie X., Wan Y.
EBIOMEDICINE, vol.44, pp.98-111, 2019 (SCI-Expanded)
- VIII. **Directionality of dynein is controlled by the angle and length of its stalk**
Can S., Lacey S., Gür M., Carter A. P., Yildiz A.
NATURE, vol.566, no.7744, pp.407-424, 2019 (SCI-Expanded)
- IX. **Why protein conformers in molecular dynamics simulations differ from their crystal structures: a thermodynamic insight**
Pullara F., Wenzhi M., Gur M.
TURKISH JOURNAL OF CHEMISTRY, vol.43, no.2, pp.394-408, 2019 (SCI-Expanded)
- X. **Molecular dynamics simulations of site point mutations in the TPR domain of cyclophilin 40 identify conformational states with distinct dynamic and enzymatic properties**
Gür M., Blackburn E. A., Ning J., Narayan V., Ball K. L., Walkinshaw M. D., Erman B.
JOURNAL OF CHEMICAL PHYSICS, vol.148, no.14, 2018 (SCI-Expanded)
- XI. **Effect of Dimerization on the Dynamics of Neurotransmitter:Sodium Symporters**
Gur M., Cheng M. H., Zomot E., BAHAR I.
JOURNAL OF PHYSICAL CHEMISTRY B, vol.121, no.15, pp.3657-3666, 2017 (SCI-Expanded)
- XII. **Energy landscape of LeuT from molecular simulations**
Gur M., ZOMOT E., CHENG M. H., BAHAR I.
JOURNAL OF CHEMICAL PHYSICS, vol.143, no.24, 2015 (SCI-Expanded)
- XIII. **Interplay between arginine methylation and ubiquitylation regulates KLF4-mediated genome stability and carcinogenesis**
Hu D., Gur M., ZHOU Z., GAMPER A., HUNG M., FUJITA N., LAN L., Bahar I., WAN Y.
NATURE COMMUNICATIONS, vol.6, 2015 (SCI-Expanded)
- XIV. **Microseconds Simulations Reveal a New Sodium-binding Site and the Mechanism of Sodium-coupled Substrate Uptake by LeuT**
Zomot E., Gur M., BAHAR I.
JOURNAL OF BIOLOGICAL CHEMISTRY, vol.290, no.1, pp.544-555, 2015 (SCI-Expanded)
- XV. **Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model**
Das A., Gur M., Cheng M. H., Jo S., Bahar I., Roux B.
PLOS COMPUTATIONAL BIOLOGY, vol.10, no.4, 2014 (SCI-Expanded)
- XVI. **Global Transitions of Proteins Explored by a Multiscale Hybrid Methodology: Application to Adenylate Kinase**
Gur M., Madura J. D., BAHAR I.
BIOPHYSICAL JOURNAL, vol.105, no.7, pp.1643-1652, 2013 (SCI-Expanded)
- XVII. **Global motions exhibited by proteins in micro- to milliseconds simulations concur with anisotropic network model predictions**
Gur M., ZOMOT E., BAHAR I.
JOURNAL OF CHEMICAL PHYSICS, vol.139, no.12, 2013 (SCI-Expanded)
- XVIII. **Computational Design of New Peptide Inhibitors for Amyloid Beta (A beta) Aggregation in Alzheimer's Disease: Application of a Novel Methodology**
Eskici G., Gur M.
PLOS ONE, vol.8, no.6, 2013 (SCI-Expanded)
- XIX. **Quasi-harmonic fluctuations of two bound peptides**
Gur M., Erman B.
PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS, vol.80, no.12, pp.2769-2779, 2012 (SCI-Expanded)

- XX. **Combining Optimal Control Theory and Molecular Dynamics for Protein Folding**
Arkun Y., Gur M.
PLOS ONE, vol.7, no.1, 2012 (SCI-Expanded)
- XXI. **Pre-existing soft modes of motion uniquely defined by native contact topology facilitate ligand binding to proteins**
Meireles L., Gur M., BAKAN A., BAHAR I.
PROTEIN SCIENCE, vol.20, no.10, pp.1645-1658, 2011 (SCI-Expanded)
- XXII. **Quasi-harmonic analysis of mode coupling in fluctuating native proteins**
Gur M., Erman B.
PHYSICAL BIOLOGY, vol.7, no.4, 2010 (SCI-Expanded)
- XXIII. **Anharmonicity, mode-coupling and entropy in a fluctuating native protein**
Kabakcioglu A., Yuret D., Gur M., Erman B.
PHYSICAL BIOLOGY, vol.7, no.4, 2010 (SCI-Expanded)
- XXIV. **Statistical thermodynamics of residue fluctuations in native proteins**
Yogurtcu O. N., Gur M., Erman B.
JOURNAL OF CHEMICAL PHYSICS, vol.130, no.9, 2009 (SCI-Expanded)

Articles Published in Other Journals

- I. **Experimental and Theoretical Investigation of Pumpkin Drying in Fluidized Bed Dryer**
GÜR M.
Uludağ University Journal of The Faculty of Engineering, vol.21, no.2, pp.145, 2016 (Peer-Reviewed Journal)
- II. **Balkabağının Akışkan Yataklı Kurutucuda Kurutulmasının Deneysel ve Teorik İncelenmesi**
Gür M.
ULUDAĞ ÜNİVERSİTESİ MÜHENDİSLİK FAKÜLTESİ DERGİSİ, vol.21, no.2, pp.145-158, 2016 (Peer-Reviewed Journal)

Supported Projects

Gür M., TÜBA Project, Nörolojik ilaçlara hedef olan hücre zarı proteinlerinin işlevinde hücre zarının etkisi, 2016 - Continues

Gür M., TUBITAK Project, Sitoplazmik dinein motor proteininin mekanokimyasal döngüsünün mekanik ve enerjetik açıdan modellenmesi, 2016 - Continues

Gür M., Project Supported by Higher Education Institutions, Sitoplazmik dinein motor proteininin mekanokimyasal çevriminin mekanizmasının modellenmesi, 2021 - 2022

Gür M., Project Supported by Higher Education Institutions, Siklofilin 40 Enziminin Termodinamik Özelliklerine Mutasyon ve Peptid Bağlanması Etkilerinin Modellenmesi, 2018 - 2020

Gür M., Project Supported by Higher Education Institutions, Çoklu Ölçekli Simülasyonlardan Elde Edilen Leut Dinamiği Bilgisi, 2015 - 2018

Gür M., Project Supported by Higher Education Institutions, SİTOPLAZMİK DİNEİN MOTOR PROTEİNİNİN MEKANOKİMYASAL DÖNGÜSÜNÜN MEKANİK VE ENERJİK AÇIDAN MODELLENMESİ, 2015 - 2016

Activities in Scientific Journals

Journal of Molecular Graphics and Modelling, Committee Member, 2016 - Continues

Metrics

Publication: 56
Citation (WoS): 391
Citation (Scopus): 398
H-Index (WoS): 9
H-Index (Scopus): 10

Congress and Symposium Activities

5. Uluslararası BAU İlaç Tasarımı Kongresi, Invited Speaker, İstanbul, Turkey, 2016

Scholarships

Nature Travel Grant, Other International Organizations, 2010 - Continues

Non Academic Experience

University of Pittsburgh