November 2023

CURRICULUM VITAE

MERT GUR

Executive Director, Computational Biomedicine & Biotechnology M.S. Program
Department of Computational & Systems Biology
School of Medicine, University of Pittsburgh
Associate Professor, Mechanical Engineering Department
School of Mechanical Engineering, Istanbul Technical University
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SHORT BIOGRAPHY

Assoc. Prof. Mert Gur is the Executive Director of the Computational Biomedicine & Biotechnology M.S. Program at the University of Pittsburgh (Pitt) School of Medicine (SOM) and a tenured faculty at Istanbul Technical University (ITU) Mechanical Engineering (ME) Department. He earned his B.S. in ME (2006) and Ph.D. in Computational Science and Engineering (2010). His research focuses on Computational Structural Biology, Computational Biomedicine, and Mechanical Engineering. Dr. Gur boasts 16+ years of experience in biomolecular simulations and modelling gathered in various top academic and research institutions in Turkey and US. He published 30+ papers in prestigious journals including Nature, Science and Nature Communications. He's been a principal investigator in 19 grants, spanning Turkey, US, and EU. His extensive leadership includes a total of five years of Vice Dean for undergraduate and graduate education at ITU. Dr. Gur taught over 42 courses to 2,500+ students at ITU and many more in Pitt ME undergraduate and SOM graduate programs. He received several awards in Turkey.

EXTENDED BIOGRAPHY

Assoc. Prof. Mert Gur is the Executive Director of the Computational Biomedicine & Biotechnology (CoBB) M.S. Program at the University of Pittsburgh (Pitt) School of Medicine (SOM) Department of Computational and Systems Biology (CSB) and a tenured Faculty in the Istanbul Technical University (ITU) Mechanical Engineering Department (ME). He earned his B.S. degree from the Middle East Technical University ME in 2006, attended the ME M.S. program at Koç University from 2006 to 2007, and completed his Ph.D. degree in Computational Science and Engineering at Koc University in 2010. He began working as postdoctoral associate in the Pitt SOM CSB, and in 2012, he was jointly appointed as a Lecturer in the Pitt Department of Mechanical Engineering and Material Science. In 2014, he joined Lawrence Berkeley National Laboratory Joint Center for Artificial Photosynthesis as a postdoctoral fellow. He became a faculty member of ITU ME at the rank of Assist. Prof. in 2015, was promoted to Assoc. Prof. in 2021, and received his tenure in 2022. Throughout summers 2016 and 2017, he was a Visiting Faculty Scholar in Pitt SOM and in the University of California Berkeley College of Chemistry. In 2022, he took a sabbatical leave from ITU ME to join the Pitt SOM CSB as a Visiting Assoc. Prof., and assumed the role of Executive Director of the CoBB M.S. Program in 2023.

Dr. Gur has held multiple leadership positions. He served as Vice Dean of the Graduate School of Science, Engineering, and Technology from 2018 to 2020 and as the Vice Dean School of Mechanical Engineering (SME) from 2020 to 2022. He simultaneously carried out both roles for six months in 2020, accumulating nearly five years of Vice Dean experience. Furthermore, he has been a member of 19 different commissions and acted as the coordinator and vice coordinator of mechanical engineering minor and double major programs at ITU. He also holds positions as the Advisory Committee Member of the National High Performance Computing Center and Board of Directors Member of the Research and Application Center for Critical and Functional Materials, and is an Elected Member Faculty Board Member of SME at ITU. In 2022 he stepped down from the ITU SME Vice Dean position to join Pitt, where he is currently leading the Pitt CoBB Program.

Dr. Gur possesses extensive teaching and mentoring experience. From 2015 to 2022, he taught 42 courses to 2,528 students across nine undergraduate and four graduate programs at ITU, averaging six courses and 361 students per year. In the US, he taught at Pitt MEMS in 2012 and has been teaching at Pitt CSB since 2023. Mert has mentored nine M.S. and 20 undergraduate students across a wide range of undergraduate and graduate programs including Molecular Biology-Genetics and Biotechnology, Mechanical Engineering, Thermal and Fluid Sciences, and Materials and Manufacture. He is currently mentoring one undergraduate, three M.S. and five Ph.D. students.

Mert brings over 16 years of experience and a proven record of innovation in applying molecular dynamics (MD) simulations and coarse-grained elastic network models to address cutting-edge scientific challenges in biology, biotechnology, biomedicine, and pharmaceutical and health sciences. His expertise spans a wide range of protein classes, such as enzymes, motors, and membrane proteins, as well as peptide design, and includes development of novel methods for enhanced sampling and free-energy calculation. Mert excels in conducting MD simulations of large biomolecular systems (up to multimillion-atoms), performing simulations with lengths several orders longer than typical, and handling big data generated by such simulations. His extensive experience in analyzing large datasets, protein-protein interactions, and designing peptide-based drugs has further solidified his standing in the field. To date, Mert and his research group have performed over 350 M core hours of MD simulations at premier Tier-0 supercomputers, including Anton and Summit (USA), Mahti (Finland), and Marconi100 (Italy).

Mert Gur acted as a principal investigator (PI)/co-PI in 19 scientific projects, consisting of 11 Turkey funded, three USA funded, and two European Union (EU) funded, and one internationally funded grants and secured a total of $2,338,775 worth of external and $30,596 of internal funding, either as direct budget or high-performance computing products and services. He also participated as researcher and co-investigator in nationally and internationally funded projects, including NIH and ANSO funded projects. So far, Mert Gur published two book chapters and more than 30 journal papers including those published in prominent journals such *Nature*, *Science*, and *Nature Communications*. Mert was awarded with multiple awards and honors, including, Outstanding Young Scientist Award (Turkish Academy of Sciences) in 2016, Young Scientist Award (Science Academy) and National Outstanding Researcher Fellowship (TUBITAK) in 2022 and Health Institutes of Türkiye (TÜSEB) Aziz Sancar Incentive Award in 2023. He is currently nominated for Associate Membership of the Turkish Academy of Sciences.

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EDUCATION AND TRAINING

UNDERGRADUATE

2006 **B.S., Mechanical Engineering**, Middle East Technical University, Ankara, Turkey

GRADUATE

2006 – 2007 Attended **M.S.** Program for a Year**, Mechanical Engineering**, Koc University, Istanbul, Turkey

2010 **Ph.D.**, **Computational Sciences and Engineering**, Koc University, Istanbul, Turkey
Delivered the Valedictorian Speech at the graduation ceremony

POSTGRADUATE

2010 – 2014 **Postdoctoral Associate**, Department of Computational and Systems Biology, **School of Medicine**, University of Pittsburgh, Pittsburgh, PA

2014 – 2015 **Postdoctoral Fellow**, Joint Center for Artificial Photosynthesis, **Lawrence Berkeley National Laboratory**-University of California, Berkeley, CA

AS FACULTY MEMBER

2022 -2023 **Springboard Program for New Faculty Investigators,** Office of Academic Career Development, **Health Sciences**, University of Pittsburgh, Pittsburgh, PA

APPOINTMENTS AND POSITIONS

2023 –Present **Executive Director**, Computational Biomedicine & Biotechnology (CoBB) M.S. Program**,** Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh

2022 –Present **Visiting Associate Professor**, Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh

2021 – Present **Faculty Board Elected Member**, Mechanical Engineering Department, School of Mechanical Engineering, Istanbul Technical University (ITU), Istanbul, Turkey

2021 – Present **Associate Professor with Tenure**, Mechanical Engineering Department, ITU (Currently on Sabbatical Leave), *Mert Gur received his tenure in 2022.*

2021 – Present **Director,** Coal and Biomass Combustion and Gasification Laboratory

2020 – 2022 **Vice Dean**, School of Mechanical Engineering, ITU
For seven months (April-November 2020) Mert Gur held both the Vice Dean positions of the School of Mechanical Engineering and the Graduate School of Science, Engineering and Technology simultaneously.

2020 – Present **Board of Directors Member**, Research and Application Center for Critical and Functional Materials, ITU, Istanbul, Turkey

2018 – 2020 **Vice Dean**, Graduate School of Science, Engineering and Technology, ITU

2019 – Present **Advisory Committee Member and Business Development Advisor to the Director**

	National Center for High Performance Computing (UHeM), ITU
2019	**Lecturer**, Council of High Education - Basic Sciences Programs Outstanding Achievement Program (YOK - TEBIP), Istanbul University , Istanbul, Turkey
2017	**Visiting Scholar,** Department of Chemistry, College of Chemistry, University of California, Berkeley, Host: Prof. Omar M. Yaghi
2016	**Visiting Faculty Scholar,** Department of Computational and Systems Biology School of Medicine, University of Pittsburgh, Host: Prof. Ivet Bahar
2015 – Present	**Academic Staff,** Department of Molecular Biology-Genetics and Biotechnology, Graduate School of Science, Engineering and Technology
2015 – Present	**Founder and Director,** Biomolecular Engineering Laboratory, ITU
2015 – 2021	**Assistant Professor,** Mechanical Engineering Department, ITU
2014 – 2015	**Postdoctoral Fellow,** Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, University of California, Berkeley
2010 – 2014	**Postdoctoral Associate**, Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh
2012	**Lecturer,** Department of Mechanical Engineering and Material Science Swanson School of Engineering, University of Pittsburgh
2007 – 2010	**Research and Teaching Assistant**, College of Engineering, Koc University
2006 – 2007	**Research and Teaching Assistant**, Department of Mechanical Engineering, College of Engineering, Koc University

UNIVERSITY SERVICES AND OTHER APPOINTMENTS

UNIVERSITY OF PITTSBURGH

2023 – Present	**Associate Director,** Training and Experimentation in Computational Biology (TECBio) Research Experiences for Undergraduates (REU) Program
2023 – Present	**Admissions committee,** Joint Carnegie Mellon-University of Pittsburgh Ph.D. Program in Computational Biology
2023 – Present	**Admissions Reviewer/screener,** Computational Biomedicine & Biotechnology M.S. Program

ISTANBUL TECHNICAL UNIVERSITY

2022 – Present	**Academic Board Member**, Materials and Manufacture Graduate Program
2021 – Present	**Member**, University Rankings and Performance Assessment Office
2021 – 2022	**Member**, International Relations Committee
2021 – 2022	**Member**, School of Mechanical Engineering International Relations Committee
2020 – 2022	**Member,** Quality Commission
2020 – 2022	**Member,** School of Mechanical Engineering Quality Commission
2020 – 2022	**Member,** Erasmus Commission
2020 – 2021	**Member**, International Ranking Unit
2019 – 2021	**Member**, Scientific Research Projects (BAP) Commission
2018 – 2020	**Member**, Internationalization Strategy Working Group
2018 – 2020	**Member**, Inter-Institute Automation Implementation Commission
2018 – 2022	**Member,** Health and Engineering Sciences Human Research Ethics Committee
2018 – 2019	**Member**, Commission for Online Teaching of Common Courses
2017 – 2020	**Coordinator**, Mechanical Engineering Minor Program
2017 – 2020	**Vice-Coordinator,** Mechanical Engineering Double Major Program
2017 – Present	**Academic Board Member**, Molecular Biology, Genetics and Biotechnology

	Graduate Program
2017 – Present	**Member**, School of Mechanical Engineering Promotion/Advertisement Committee
2015 – 2022	**Member,** Mechanical Engineering Program Quality Assurance and ABET Committee
2015 – 2020	**Associate Head**, Mechanical Engineering Faculty Transfer and Adaptation Committee
2015 – Present	**Academic Board Member**, Heat-Fluid (Thermal and Fluid Sciences) Graduate Program
2015 – Present	**Academic Board Member**, Mechanical Engineering Graduated Program

AWARDS AND HONORS

2023	**Aziz Sancar Incentive Award**, Health Institutes of Turkey (TUSEB)
2023	**Nominated for Associate Membership,** Turkish Academy of Sciences (Result to be announced)
2023	**Academic Performance Award,** Istanbul Technical University
2022	**2247-A National Outstanding Researchers Program,** The Scientific and Technological Research Council of Turkey (TUBITAK)
2022	**Young Scientist Awards Program** (BAGEP)**,** The Science Academy (Bilim Akademisi)
2021	**Work featured on cover** of *The Journal of Physical Chemistry B*
2017	**Invited Participant**, World Science Forum
2017	**Accommodation Grant,** World Science Forum
2016	**Outstanding Young Scientist Award** (GEBIP), TUBA
2015	**2232-Research Fellowship Program for Outstanding Scientist** Returning to Turkey, TUBITAK
2013	**Work featured on cover** of *Biophysical Journal*
2011	**Work featured on cover** of *Protein Science*
2010	**Nature Publishing Group Award,** Award covered travel and registration expenses to the Biopolymers Gordon Research Conference
2010	**Gave Valedictorian Speech** at the Koc University graduation ceremony

TEACHING

COURSES TAUGHT

UNIVERSITY OF PITTSBURGH

Integrative Systems Biology Ph.D. program

Computational Biomedicine and Biotechnology M.S. Program

Fall 2023	MSCBIO 2025	Introduction to Bioinformatics Programming in Python *Partial Teaching*	18 Students

Computational Biomedicine and Biotechnology M.S. Program

Fall 2023	CoBB 2010	Foundations in Computational Biology	5 Students

Joint Carnegie Mellon-University of Pittsburgh Ph.D. Program in Computational Biology

Spring 2023	MSCBIO 2041	Cellular & Systems Modeling *Partial Teaching*	20 Students

Mechanical Engineering Undergraduate Program

Spring 2012	MEMS 1065	Thermal Systems Design	50 Students

ISTANBUL TECHNICAL UNIVERSITY

Mechanical Engineering Undergraduate Program

Spring 2022	DAN 102	Entrepreneurship and Career Counselling	377 Students
Spring 2022	MAK 4079	Thermodynamics of Biomolecular Systems	18 Students
Fall 2021	DAN 101	Academic Advising	76 Students
Spring 2021	DAN 301	Career Advising	247 Students
Spring 2021	MAK 4079	Thermodynamics of Biomolecular Systems	89 Students
Fall 2020	DAN 101	Academic Advising	247 Students
Spring 2020	MAK 215	Thermodynamics I	88 Students
Spring 2020	MAK 4079	Thermodynamics of Biomolecular Systems	26 Students
Fall 2019	MAK 211E	Probability and Statistics	82 Students
Fall 2019	MAK 215	Thermodynamics I	83 Students
Spring 2019	MAK 226	Thermodynamics II	75 Students
Fall 2018	MAK 215	Thermodynamics I	93 Students
Fall 2018	MAK 211E	Probability and Statistics	74 Students;
Spring 2018	TER 206	Thermodynamics II	53 Students
Fall 2017	TER 205	Thermodynamics I	71 Students
Spring 2017	BIO 102	Engineering Biology	129 Students
Fall 2016	TER 201E	Thermodynamics	54 Students
Fall 2016	MAK 370	Applied Heat Transfer	40 Students
Spring 2016	BIO 102	Engineering Biology	136 Students
Fall 2015	BIO 102	Engineering Biology	38 Students
Manufacturing Engineering Undergraduate Program			
Spring 2018	MAK 218	Thermodynamics and Heat Conduction	56 Students
Spring 2017	MAK 218	Thermodynamics and Heat Conduction	46 Students
Spring 2016	MAK 218	Thermodynamics and Heat Conduction	28 Students
Mineral Processing Engineering, Petroleum and Natural Gas Engineering, Management Engineering, Textile Engineering, Shipbuilding and Ocean Engineering, Environmental Engineering, Bioengineering Undergraduate Programs			
Summer 2019	TER 201E	Thermodynamics	10 Students
Fall 2017	TER 201E	Thermodynamics	58 Students
Fall 2016	TER 201E	Thermodynamics	54 Students
Fall 2015	TER 201E	Thermodynamics	51 Students
Heat-Fluid (Fluid and Thermal Sciences) M.S. Program			
Spring 2021	MIA 504	Advanced Heat and Mass Transfer	5 Students
Spring 2020	MIA 504	Advanced Heat and Mass Transfer	11 Students
Molecular Biology-Genetics and Biotechnology M.S. Program			
Fall 2021	MBG 532	Bioinformatics	16 Students
Spring 2021	MBG 535	Laboratory Research	1 Student
Spring 2020	MBG 535	Laboratory Research	1 Student
Fall 2020	MBG 532	Bioinformatics	28 Students
Fall 2019	MBG 532	Bioinformatics	16 Students
Spring 2019	MBG 535	Laboratory Research	3 Students
Fall 2018	MBG 532	Bioinformatics	11 Students
Spring 2018	MBG 535	Laboratory Research	3 Students
Fall 2017	MBG 532	Bioinformatics	18 Students
Molecular Biology-Genetics and Biotechnology Ph.D. Program			
Fall 2020	MBG632	Guided Research	1 Student

Mechanical Engineering Ph.D. Program

Fall 2021	MAK 692E	Statistical Thermodynamics of Thermal Systems	3 Students
Fall 2020	MAK 692E	Statistical Thermodynamics of Thermal Systems	6 Students
Spring 2019	MAK 692E	Statistical Thermodynamics of Thermal Systems	6 Students

ISTANBUL UNIVERSITY

YOK-Basic Sciences Programs (TEBIP) for Outstanding Students

Spring 2019	TEBKP1-2	Personal Project I	1 Student

NEW COURSES CONTRIBUTED TO UNDERGRADUATE AND GRADUATE PROGRAMS

ISTANBUL TECHNICAL UNIVERSITY

Mechanical Engineering Undergraduate Program

2022	MAK 4080E	Fundamentals and Applications of Nanomachines
2019	MAK 4079	Thermodynamics of Biomolecular Systems

Mechanical Engineering Ph.D. Program

2018	MAK 692E	Statistical Thermodynamics of Thermal Systems

NEW CURRICULUM DEVELOPMENT

ISTANBUL TECHNICAL UNIVERSITY

Mechanical Engineering Undergraduate Program

2021 As the School of Mechanical Engineering Vice Dean for Academic Affairs, I developed a revised mechanical engineering curriculum. The updated curriculum has been effective since 2021. https://www.sis.itu.edu.tr/EN/student/undergraduate/courseplans/plans/MAK/202210.html

TEACHING IN WORKSHOPS AND SUMMER PROGRAMS

2023 Journal Club, Training and Experimentation in Computational Biology (TECBio), undergraduate students.

2022 Hands on session, CCPBioSim Training Week 2022-Workshop on ProDy, graduate students

MENTORING OF GRADUATE AND UNDERGRADUATE STUDENTS

Ph.D. Students

Istanbul Technical University, Molecular Biology-Genetics and Biotechnology Department

2023 – Present	Ayla Eren, Molecular Biology-Genetics and Biotechnology Program
2022 – Present	Clara Xazal Buran, Molecular Biology-Genetics and Biotechnology Program
2022 – Present	Reyhan Metin Akkaya, Molecular Biology-Genetics and Biotechnology Program
2020 – Present	Mert Gölcük, Molecular Biology-Genetics and Biotechnology Program
2020 – 2022	Elhan Taka, Biology-Genetics and Biotechnology Program
2020 – Present	Sema Zeynep Yılmaz, Biology-Genetics and Biotechnology Program

M.S. Students

Istanbul Technical University, Molecular Biology-Genetics and Biotechnology Department

2022 – Present	Ebru Tuncay, Molecular Biology-Genetics and Biotechnology Program
2022 – Present	Cihan Uğur Otçu, Molecular Biology-Genetics and Biotechnology Program
2022 – 2022	Ayten Dilara Gürsel, Molecular Biology-Genetics and Biotechnology Program
2020 – 2022	Clara Xazal Buran, Molecular Biology-Genetics and Biotechnology Program
2022 – 2020	Onur Özer, Molecular Biology-Genetics and Biotechnology Program

2020 – 2018 Ceren Kılınç, Molecular Biology-Genetics and Biotechnology Program
2020 – 2018 Mert Gölcük, Molecular Biology-Genetics and Biotechnology Program
2020 – 2018 Elhan Taka, Molecular Biology-Genetics and Biotechnology Program
2020 – 2018 Sema Zeynep Yılmaz, Molecular Biology-Genetics and Biotechnology Program

Istanbul Technical University, Department of Mechanical Engineering

2022 – 2023 Mert Kemal Doğru, Materials and Manufacture Graduate Program
2022 – 2018 Halil Kaya, Heat-Fluid M.S. Program
2020 – Present Emre Fındık, Heat-Fluid Graduate Program
2019 – 2017 Mohammad Amin Salehi Tabrizi, Heat-Fluid M.S. Program

Undergraduate Students

Istanbul Technical University

2022 – Present Kübra Nur Çil, Molecular Biology and Genetics Program
2022 – 2023 Zafer Akpınar, Mechanical Engineering Program
2022 – 2022 Öykü Çelik, Molecular Biology and Genetics Program
2021 – 2021 Gani Şen, Molecular Biology and Genetics Program
2020 – Present Derman Baştürk, Mechanical Engineering Program
2020 – 2021 Gamze Saçmaözü, Mechanical Engineering Program
2020 – 2021 Direnç Akyıldız, Mechanical Engineering Program
2020 – 2021 Yaren Barutçu, Mechanical Engineering Program
2019 – 2019 Serkan İlter, Manufacturing engineering Program
2019 – 2019 Mustafa Can Ersoy, Manufacturing engineering Program
2019 – 2019 Rıdvan Ak, Manufacturing engineering Program
2016 – 2019 Orhan Sadi, Mechanical Engineering Program
2016 – 2019 Ayça Kepçe, Electronics and Communication Engineering Program
2016 – 2019 Ali Burak Aşçı, Mechanical Engineering Program
2016 – 2018 Şafak Muratoğlu, Metallurgical and Materials Engineering
2016 – 2018 Mirza Özdil, Mechanical Engineering Program
2016 – 2018 Gözde Büyükaçıkgül Muratoğlu, Manufacturing Engineering Program
2015 – 2016 Berkay Günay, Mechanical Engineering Program
2015 – 2016 Oktay Çelik, Mechanical Engineering Program
2015 – 2016 Meriç Aras, Mechanical Engineering Program

Istanbul University

2016 – 2018 Nilüfer Toker, YOK-Basic Sciences Programs Outstanding Classes (TEBIP), Biology Program

Koc University

2020 – 2021 Hasan Tuncer, Physics and Electrical-Electronics Engineering Program

SERVICE ON THESIS COMMITTEES

(Date of Defense or Proposal Given)

CARNEGIE MELLON UNIVERSITY AND UNIVERSITY OF PITTSBURGH

December 2022	PhD Student	Haotian Zhang	Joint Carnegie Mellon-University of Pittsburgh Ph.D. Program in Computational Biology

ISTANBUL TECHNICAL UNIVERSITY

September 2022	Ph.D. student	Ezgi Baştürk	Molecular Biology-Genetics and Biotechnology
September 2022	Ph.D. student	Baran Dingiloğlu	Molecular Biology-Genetics and Biotechnology
September 2022	Ph.D. student	Nisan Denizce	Molecular Biology-Genetics and Biotechnology

September 2022	Ph.D. student	Miray Türk	Molecular Biology-Genetics and Biotechnology
September 2022	Ph.D. student	Jale Yıldız	Molecular Biology-Genetics and Biotechnology
September 2018	Ph.D. student	Özge Tatlı	Molecular Biology-Genetics and Biotechnology

BAHCESEHIR UNIVERSITY

September 2020	M.S. student	Lalehan Oktay	Bioengineering
September 2020	M.S. student	Asena Himmetoğlu	Neuroscience Master Program

BOGAZICI UNIVERSITY

December 2019	M.S. student	Emir Kocer	Mechanical Engineering Program
March 2017	Ph.D. student	Tolga Akiner	Mechanical Engineering program

KOC UNIVERSITY

January 2023	Ph.D. student	M. Tuğrul Birtek	Mechanical Engineering
December 2019	M.S. student	Fulya Akşit	Chemical and Biological Engineering Program
July 2019	M.S. student	Meltem Eda Omur	Molecular Biology and Genetics Program
September 2018	Ph.D. student	Emine Sıla Özdemir	Chemical and Biological Engineering
March 2016	Ph.D. student	Mohammed Adamu Isa	Mechanical Engineering
March 2016	Ph.D. student	Syed Shahid Mustafa	Biomedical Engineering program

SABANCI UNIVERSITY

December 2021	Ph.D. student	Işık Kantarcıoğlu	Molecular Biology, Genetics and Bioengineering
December 2021	Ph.D. student	Ebru Çetin	Materials Science and Nano Engineering

STUDENT CLUB ADVISING SERVICE

2017 – Present Istanbul Technical University Fitness Club Advisor

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RESEARCH

GRANTS

PRINCIPAL INVESTIGATOR (PI)

18. Self-Coordination of Dyneins During Ciliary Beating
    Project Role: PI
    Funding Source: TUBITAK (The Scientific and Technological Research Council of Turkey)
    Project Budget: 900,000 TL (~$49,247), The grant provides stipends for three graduate students.
    Project No: 122N045 (2501 - Joint Research Program with National Science Foundation (NSF))
    Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), graduate and undergraduate students
    Project Date: 2022- 2025

17. Molecular-Scale Modeling of Dynein Microtubule Binding and Power Stroke
    Project Role: PI
    Funding Source: TUBITAK
    Project Budget: 2,474,000 TL (~$133,951.4), The grant provides stipends for five graduate students.
    Project No: 121C283, 2247-A National Outstanding Researcher Fellowship
    Project Team: Mert Gur, graduate students
    Project Date: 2022- 2025

16. Modeling The Regulation of Motors by Microtubule-Associated Proteins.
    Project Role: PI
    Funding Source: Partnership for Advanced Computing in Europe, PRACE (European Union)
    Project Budget: 117,662,006 standardized core-hour (~$366.415,1 worth of computational resources; *cost estimate is based on supercomputer TRUBA in Turkey*)
    Project No: 2021250119
    Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), Eva Nogales (UC Berkeley), graduate students
    Project Date: 2022-2023

15. Identification And Reengineering of Effective Nanobodies Against SARS-Cov-2 Omicron Variant
    Project Role: Co-PI
    Funding Source: COVID-19 High Performance Computing Consortium (USA)
    Project Budget: 30,000,000 standardized core-hour (~$112,801.8 worth of computational resources)
    Project No: TG-BIO210181
    Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), graduate students
    Project Dates: 2021- 2022

14. The Mechanism and Energetics of Dynein's Powerstroke (Endy)
    Project Role: PI
    Funding Source: DECI-17 (Distributed European Computing Initiative), PRACE (European Union)
    Project Budget: 11,171,484.16 standardized core-hour (~$106,554.8 worth of computational resources)
    Project No: 17DECI0080
    Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), graduate students
    Project Dates: 2021 – 2022

13. Modeling the Mechanism of the Mechanochemical Cycle of the Cytoplasmic Dynein Motor Protein
    Project Role: PI
    Funding Source: Istanbul Technical University (ITU) BAP
    Project Budget: 74.997,26 TL (~$10,257.16)
    Project No: MGA-2021-42803
    Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), graduate student
    Project Dates: 2021 – 2022

12. Designing Cell Penetrating Peptide Based Drug Candidates for Behcet's Disease
Project Role: PI
Funding Source: TUBITAK
Project Budget: 808,789 TL (~$123,296.20), The grant provides stipends for three graduate and one undergraduate student.
Project No: 119Z553 (TUBITAK 1001 Project)
Project Team: Mert Gur, Ahmet Gül (Istanbul University, Capa School of Medicine), Sema Sırma Ekmekçi, Neslihan Abacı (Istanbul University, Aziz Sancar Institute of Experimental Medicine), graduate and undergraduate students
Project Dates: 2020 – 2023

11. Development of an Early Detection System for Hereditary Colon and Breast Cancers and its Integration into e-Nabız Personal Health Record System
Project Role: PI
Funding Source: TUBITAK
Project Budget: 2,111,990.36 TL (~$378,023), This project supports five graduate and two undergraduate students.
Project No: 318S129 (TUBITAK 1003 Project)
Project Team: Mert Gur, Gizem Dinler Doğanay (ITU), undergraduate and graduate students.
Project Dates: 2020 – 2023

10. Exploring Nanobody Inhibitory Mechanism against SARS-CoV-2 Spike Glycoprotein Using Molecular Dynamics Simulations, (UC Berkeley – ITU Collaboration)
Project Role: Co-PI
Funding Source: COVID-19 High Performance Computing Consortium (USA)
Project Budget: 46,000,000.00 standardized core-hour (~$356,354.1 worth of computational resources)
Project No: TG-BIO200053
Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), graduate students
Project Dates: 2020 – 2021

9. Exploring Binding and Fusion Mechanism of SARS-CoV-2 Spike Glycoprotein Using Molecular Dynamics Simulations, (UC Berkeley – ITU Collaboration)
Project Role: Co-PI
Funding Source: COVID-19 High Performance Computing Consortium (USA)
Project Budget: 25,000,000.00 standardized core-hour (~$310,060.1 worth of computational resources)
Project No: TG-MCB200070
Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), graduate students
Project Dates: 2020 – 2021

8. Modelling the Mechanochemical Cycle of Cytoplasmic Dynein Machinery
Project Role: PI
Funding Source: Partnership for Advanced Computing in Europe, PRACE (European Union)
Project Budget: 48,400,000.00 standardized core-hour (~ $211,959.6 worth of computational resources)
Project No: 2019215144
Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), Andrew P. Carter (MRC Laboratory of Molecular Biology), graduate student
Project Dates: 2020 – 2021

7. Exploring Differences In Binding Characteristics Between HLA-B51 And HLA-B52
   Project Role: PI
   Funding Source: NVIDIA Hardware Grant Program
   Project Budget: NVIDIA TitanV GPU, ~3,000$
   Project Team: Mert Gur, graduate students
   Project Dates: 2019 – 2019

6. Modeling the Effects of Mutation and Peptide Binding on Thermodynamic Properties of Cyclophilin 40 Enzyme
   Project Role: PI
   Funding Source: Istanbul Technical University BAP
   Project Budget: 50,000 TL (~$14,411.48)
   Project No: MGA-2018-41072
   Project Team: Mert Gur, graduate students
   Project Dates: 2018 – 2019

5. Effect of Cell Membrane on the Function of Membrane Proteins Targeted by Therapeutic Drugs Against Neurological Disorders
   Role: PI
   Funding Source: Turkish Academy of Science (TUBA)
   Project Budget: 60,000 TL (~$19,339.86)
   Project No: 2016 TUBA GEBİP Award
   Project Team: Mert Gur, graduate students
   Project Dates: 2016 – 2019

4. Insight To Leut Dynamics Obtained from Multi-Scale Simulations
   Project Role: PI
   Funding Source: ITU BAP
   Project Budget: $2,148 (Travel Grant)
   Project No: 38588 (Link- International Collaboration Support Program)
   Project Dates: 2016 Summer

3. Modeling the Mechanics and Energetics of the Cytoplasmic Dynein Motor Protein Mechanochemical Cycle
   Project Role: PI
   Funding Source: TUBITAK
   Project Budget: 357,006 TL (~ $126,208.51), This project supported three graduate and one undergraduate students.
   Project No: 215Z398 (TUBITAK 3501 Project)
   Project Team: Mert Gur, Ahmet Yildiz (UC Berkeley), undergraduate and graduate students.
   Project Dates: 2016 – 2019

2. Mechanical and Energetic Modeling of the Mechanochemical Cycle of the Cytoplasmic Dynein Motor Protein
   Project Role: PI
   Funding Source: ITU BAP
   Project Budget: $3,780 (Travel Grant)
   Project No: 38777 (International Research Collaboration Project)
   Project Dates: 2015 Summer

1. Investigation and Modeling of Functional Mechanisms of Cell Membrane Proteins Targeting Neurological Drugs
   Project Role: PI
   Funding Source: TUBITAK
   Project Budget: 128,000 TL (~ $41,327)
   Project No: 115C038 (TUBITAK 2232 Research Fellowship for Outstanding Scientist Returning to Turkey)
   Project Dates: 2015 – 2017

COLLABORATOR/ RESEARCHER/ EXPERT

5. Toward a Deeper Understanding of Allostery and Allotargeting by Computational Approaches
   Project Role: Researcher
   Funding Source: National Institutes of Health (NIH)
   Project Budget: $ 348,183.00
   Project No: 5R01GM139297-02
   Project Team: Mert Gur, Ivet Bahar (PI), Pemra Doruker (co-PI)
   Project Dates: 2021 – 2025

4. A First Step Valorization of Waste Atmospheric Carbon Dioxide via its Sustainable Capture
   Project Role: Collaborator
   Funding Source: Alliance of International Science Organizations, ANSO (International)
   Project Budget: $150,000.00
   Project No: ANSO-CR-PP-2020-06
   Project Team: Mert Gur, Bassem Al-Maythalony (PI) (Royal Scientific Society, Jordan), Yuebiao Zhang (ShanghaiTech University, China), Youssef Belmabkhout (Mohammed VI Polytechnic University, Morocco, Jordan) Karim Adil (Le Mans University, France), Gamze Gumuslu Gur (ITU)
   Project Dates: 2021 – 2024

3. Turkey's Spatial Strategic Plan Preparation and Strategic Environmental Assessment Project
   Project Role: Energy Expert
   Funding Source: Republic of Turkey Ministry of Environment and Urbanization
   Project Budget: $63,163.21 (II. stage) and $555,856.44 (III. stage)
   Project No: TMSP II. Etap (2020) and TMSP III. Etap (2021)
   Project Team: 34 experts (II. stage) and 40 experts (III. stage) from Istanbul Technical, Istanbul, Arel, Kent and Ege Universities
   Project Dates: 2020 – 2021

2. Design and Application of SARS-CoV-2 Viral Spike (S) Protein and ACE2 inhibitors for the Treatment of Covid-19 Disease
   Project Role: Researcher
   Funding Source: TUBITAK
   Project Budget: $55,303.60
   Project No: 120Z305 (TUBITAK 1001 Project)
   Project Team: Mert Gur, Gizem Dinler Doğanay (PI), Sefer Baday
   Project Dates: 2020 – 2021

1. Additive Manufacturing Research Center (EKAM)
   Project Role: Researcher
   Funding Source: Istanbul Development Agency's 2018 Innovative and Creative Istanbul Financial Support Program
   Project Budget: $357,004.87
   Project No: TR10/18/YMP/0005
   Project Team: 17 ITU and one Marmara University Faculty Members
   Project Dates: 2018 – 2020

GRANTS IN WHICH MERT GUR PARTICIPATED DURING POSTDOCTORAL TRAINING

6. Joint Center for Artificial Photosynthesis
   Institution: Lawrence Berkeley National Laboratory, University of California, Berkeley
   Postdoctoral Advisor: Teresa Head-Gordon
   Funding Source: U.S. Department of Energy (DOE)
   Project Budget: $750.000,00
   Project Role: Postdoctoral Fellow
   Dates Attended the Project: 2014 – 2015
   Project No: DE-SC0004993

5. Continued Development of Protein Dynamics Software ProDy
   Institution: Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh, Pittsburgh, PA, USA
   Postdoctoral Advisor: Ivet Bahar
   Funding Source: National Institutes of Health (NIH)
   Project Budget: $1,142,251
   Project Role: Postdoctoral Associate
   Dates Attended the Project: 2013 – 2014
   Project No: R01 GM099738

4. High Performance Computing for Multiscale Modeling of Biological Systems
   Institution: Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh, Pittsburgh, PA, USA
   Postdoctoral Advisor: Ivet Bahar
   Funding Source: NIH
   Project Budget: $13,394,197
   Project Role: Postdoctoral Associate
   Dates Attended the Project: 2012 – 2013
   Project No: P41 GM103712

3. Membrane Protein Structural Dynamics Consortium-Computational Modeling Resource Core
   Institution: Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh, Pittsburgh, PA, USA
   Postdoctoral Advisor: Ivet Bahar
   Funding Source: NIH
   Project Budget: $31.930,663
   Project Role: Postdoctoral Associate
   Dates Attended the Project: 2010 – 2014
   Project No: U54 GM087519

2. Structural Dynamics of Biomolecular Systems
   Institution: Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh, Pittsburgh, PA, USA
   Postdoctoral Advisor: Ivet Bahar
   Funding Source: NIH
   Project Budget: $1.309.441,00
   Project Role: Postdoctoral Associate
   Dates Attended the Project: 2010 – 2012
   Project No: R01 GM086238

1. University of Pittsburgh Clinical and Translational Science Institute-Molecular and Systems Modeling Core
   Institution: Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh, Pittsburgh, PA, USA
   Postdoctoral Advisor: Ivet Bahar
   Funding Source: NIH
   Project Budget:
   Project Role: Postdoctoral Associate
   Dates Attended the Project: 2010 – 2012
   Project No: UL1 RR024153

JOURNAL ARTICLES

34. Banerjee, A., Mathew, S., Naqvi, M. M., Yilmaz, S. Z., Zacharopoulou, M., Doruker, P., Kumita, J. R., Yang S., **Gur, M**., Itzhaki, L. S., Gordon, R., Bahar, I., Influence of Point Mutations on PR65 Conformational Adaptability: Insights from Optical Tweezer Experiments and Molecular Simulations, **Research Square** (Corresponding author) (Preprint)
33. Salvador-Garcia, D., Jin, L., Hensley, A., Golcuk, M., Gallaud, E., Chaaban, S., Port, F., Vagnoni, A., Planelles-Herrero, V.J., McClintock, M.A., Derivery, E., Carter, A.P., Giet, R., **Gur, M**., Yildiz, A., Bullock, S.L. (2023). A force-sensitive mutation reveals a spindle assembly checkpoint-independent role for dynein in anaphase progression, **bioRxiv**, 2023.08. 03.551815. (Preprint) (Currently under review)
32. Costa, M. G. S., **Gur, M**., Krieger, J. M., Bahar, I. (2023). Computational biophysics meets cryo-EM revolution in the search for the functional dynamics of biomolecular systems, **WIREs Computational Molecular Science**, 2023.06. 10.544469. (Joint First Author) (2022 Impact Factor: 11.4)
31. Golcuk, M., Yilmaz, S. Z., Yildiz, A., **Gur, M**. (2023). The Mechanism and Energetics of the Dynein Priming Stroke, **bioRxiv**, 2023.06. 10.544469. (Preprint) (Currently under review) (Corresponding Author)

30. Golcuk M., Yildiz, A., **Gur, M**. (2022). Omicron BA.1 and BA.2 Variants Increase the Interactions of SARS-CoV-2 Spike Glycoprotein with ACE2. **Journal of Molecular Graphics & Modelling,** 108286. (Corresponding Author)
29. Golcuk M., Hacisuleyman, A., Yilmaz, S. Z., Taka, E. Yildiz A., **Gur. M**. (2022). SARS-Cov-2 Delta Variant Decreases Nanobody Binding and ACE2 Blocking Effectivity. **Journal of Chemical Information and Modeling**. 62 (10), 2490-2498. (Corresponding Author)
28. Ferro, L. S., Fang, Q., Eshun-Wilson, L., Fernandes, J., Jack, A., Farrell, D. P., Golcuk, M., Huijben, T., Costa, K., **Gur, M.**, DiMaio, F., Nogales, E., Yildiz, A., (2022) Structural and functional insight into regulation of kinesin-1 by microtubule-associated protein MAP7. **Science**, 375, 326-331.
27. **Gur, M.,** Yilmaz, S. Z., Taka, E. (2021). The First Law of Thermodynamics Analysis of Transporters Involved in the Glutamate/Gaba-Glutamine Cycle. **Journal of Thermal Science and Technology**. 41(2), 265-276. (Corresponding Author)
26. Golcuk, M., Hacisuleyman, A., Erman, B., Yildiz, A., **Gur M.** (2021). Binding mechanism of neutralizing Nanobodies targeting SARS-CoV-2 Spike Glycoprotein. **Journal of Chemical Information and Modeling**. 61(10), 5152–5160. (Corresponding Author)
25. Taka, E., Yilmaz, S. Z., Golcuk, M., Kilinc, C., Aktas, U., Yildiz, A., **Gur, M**. (2021). Critical interactions between the SARS-CoV-2 spike glycoprotein and the human ACE2 receptor. **Journal of Physical Chemistry B**. 125 (21), 5537-5548. (Corresponding Author)
24. Ferro, L., Eshun-Wilson, L., Golcuk, M., Fernandes, J., Huijben, T., Gerber, E., Jack, A., Costa, K., **Gur, M.**, Fang, Q., Nogales, E. and Yildiz, A. (2020). The mechanism of motor inhibition by microtubule-associated proteins. **bioRxiv**. (Preprint)
23. **Gur, M.**, Taka, E., Yilmaz, S. Z., Kilinc, C., Aktas, U., Golcuk, M. (2020). Conformational transition of SARS-CoV-2 spike glycoprotein between its closed and open states. **Journal of Chemical Physics**, 153(7), 075101. (Corresponding Author)
22. **Gur, M**. (2020). COVID-19 aşı ve ilaç geliştirme çalışmalarında spike glikoproteininin yeri ve önemi. **TÜBA Günce**, 63.
21. **Gur, M.**, Golcuk, M., Gul, A., Erman, B. (2020). Molecular dynamics simulations provide molecular insights into the role of HLA-B51 in Behçet's Disease pathogenesis. **Chemical Biology & Drug Design**, 96(1), 644-658. (Corresponding Author)
20. Zhou, Z., Feng, Z., Hu, D., Yang, P., **Gur, M.**, Bahar, I., Cristofanilli, M., Gradishar, W.J., Xie, X., Wan, Y. (2019). A novel small-molecule antagonizes PRMT5-mediated KLF4 methylation for target therapy. **EBioMedicine- Lancet**, 44, 98-111.
19. **Gur, M.**, Golcuk, M., Yilmaz, S. Z., Taka, E. (2019). Thermodynamic first law efficiency of membrane proteins. **Journal of Biomolecular Structure & Dynamics**, 1-11. (Corresponding Author)
18. Can, S., Lacey, S., **Gur, M.**, Carter, A. P., Yildiz, A. (2019). Directionality of dynein is controlled by the angle and length of its stalk. **Nature**, 566(7744), 407.
17. Pullara, F., Wenzhi, M., **Gur, M.** (2019). Why protein conformers in molecular dynamics simulations differ from their crystal structures: a thermodynamic insight. **Turkish Journal of Chemistry**, 43(2), 394-403. (Corresponding Author)
16. **Gur, M.**, Blackburn, E. A., Ning, J., Narayan, V., Ball, K. L., Walkinshaw, M. D., Erman, B. (2018). Molecular dynamics simulations of site point mutations in the TPR domain of cyclophilin 40 identify conformational states with distinct dynamic and enzymatic properties. **Journal of Chemical Physics**, 148(14), 145101. (Corresponding Author)
15. **Gur, M.**, Cheng, M. H., Zomot, E., Bahar, I. (2017). Effect of dimerization on the dynamics of neurotransmitter: sodium symporters. **Journal of Physical Chemistry B**, 121(15), 3657-3666. (Corresponding Author)

14. **Gur, M.** (2016). Balkabağının akışkan yataklı kurutucuda kurutulmasının deneysel ve teorik incelenmesi. **Uludağ University Journal of The Faculty of Engineering**, 21(2), 145-158.
13. **Gur, M.**, Zomot, E., Cheng, M. H., Bahar, I. (2015). Energy landscape of LeuT from molecular simulations. **Journal of Chemical Physics**, 143 (24), 243134 (Corresponding Author)
12. Hu, D.*, **Gur, M.***, Zhou, Z., Gamper, A., Hung, M. C., Fujita, N., Lan L, Bahar I., Wan, Y. (2015). Interplay between arginine methylation and ubiquitylation regulates KLF4-mediated genome stability and carcinogenesis. **Nature Communications**, 6, 8419. (Joint First Author)
11. Zomot, E., **Gur, M.**, Bahar, I. (2015). Microseconds simulations reveal a new sodium-binding site and the mechanism of sodium-coupled substrate uptake by LeuT. **Journal of Biological Chemistry**, 290(1), 544-555.
10. Das, A., **Gur, M.**, Cheng, M. H., Jo, S., Bahar, I., Roux, B. (2014). Exploring the conformational transitions of biomolecular systems using a simple two-state anisotropic network model. **PLOS Computational Biology**, 10(4), e1003521.
9. **Gur, M.**, Madura, J. D., Bahar, I. (2013). Global transitions of proteins explored by a multiscale hybrid methodology: application to adenylate kinase. **Biophysical Journal**, 105(7), 1643-1652. (Featured as new and notable).
8. **Gur, M.**, Zomot, E., Bahar, I. (2013). Global motions exhibited by proteins in micro-to milliseconds simulations concur with anisotropic network model predictions. **Journal of Chemical Physics**, 139(12), 121912.
7. Eskici, G., **Gur, M.** (2013). Computational design of new peptide inhibitors for amyloid beta (Aβ) aggregation in Alzheimer's disease: application of a novel methodology. **PLOS One**, 8(6), e66178. (Corresponding Author)
6. **Gur, M.**, Erman, B. (2012). Quasi-harmonic fluctuations of two bound peptides. **Proteins: Structure, Function, and Bioinformatics**, 80(12), 2769-2779. (Corresponding Author)
5. Arkun, Y., **Gur, M.** (2012). Combining optimal control theory and molecular dynamics for protein folding. **PLOS One**, 7(1), e29628
4. Meireles, L., **Gur, M.***, Bakan, A.*, Bahar, I.* (2011). Pre-existing soft modes of motion uniquely defined by native contact topology facilitate ligand binding to proteins. **Protein Science**, 20(10), 1645-1658. (Joint first author)
3. Kabakçioğlu, A., Yuret, D., **Gur, M.**, Erman, B. (2010). Anharmonicity, mode-coupling and entropy in a fluctuating native protein. **Physical Biology**, 7(4), 046005.
2. **Gur, M.**, Erman, B. (2010). Quasi-harmonic analysis of mode coupling in fluctuating native proteins. **Physical Biology**, 7(4), 046006.
1. Yogurtcu, O. N., **Gur, M.**, Erman, B. (2009). Statistical thermodynamics of residue fluctuations in native proteins. **Journal of Chemical Physics**, 130(9), 03B607.

BOOK CHAPTERS

2. **Gur, M.** (2020) Exploring conformational transition of 2019 novel coronavirus spike glycoprotein between its closed and open states using molecular dynamics simulations. In M., Şeker, A., Özer, Z., Tosun, C., Korkut, M., Doğrul (Ed.). **TÜBA Assessment Report on COVID-19 Global Outbreak** (pp. 161). Ankara, Turkey: Turkish Academy of Sciences Publications

1. **Gur, M.**, Gur, M. (2014). Comparing Corn Drying in Fluidized Bed Dryer and Convective Tray Dryer. In I., Dincer, A., Midilli, H., Kucuk (Ed.). **Progress in Exergy Energy and the Environment** (pp. 1085). Springer International Publishing.(Corresponding author)

CONFERENCE, SYMPOSIA AND MEETING PRESENTATIONS

37. Golcuk, M., Yilmaz, S. Z., Yildiz A. **Gur M**. (2022) The Mechanism and Energetics of the Dynein Priming Stroke. **8th International BAU-Drug Design Congress**. Istanbul, Turkey
36. Buran C. H., Taka, E., **Gur M.** (2022) Investigation of The Structural Differences Between Wild-Type and Mutant Forms of Mutsa Heterodimer with Molecular Dynamic Simulations. **8th International BAU-Drug Design Congress**. Istanbul, Turkey
35. Yilmaz, S. Z., Golcuk, M., Erman, B., **Gur, M**. (2022). Modelling cell membrane passing mechanism and energetics of cell penetrating peptides comprising HLA-B*51 binding motifs. **International Congress of the Molecular Biology Association of Turkey (MolBiyoKon22).** Istanbul, Turkey
34. Dingiloglu, B., Basturk, E., Turk M., Golcuk M., Eyupoglu, A. E., Karakus, B. Z., Can O., Erman B., **Gur M**., Dinler-Doğanay, G. (2022). Developing novel Peptide-based Inhibitor Candidates against Receptor Binding Domain (RBD) of SARS-CoV-2 Spike Protein. **International Congress of the Molecular Biology Association of Turkey (MolBiyoKon22).** Istanbul, Turkey
33. **Gur, M.** (2021). Exploring conformational transitions during the CHK2 activation via molecular dynamics simulations. **3rd International Cancer and Ion Channels Congress (CANCERION-2021).** (Invited Speaker)
32. **Gur, M.**, Yilmaz, S.Z., Taka, E. (2021). Thermodynamic First Law Analysis of Transporters Involved in the Glutamate/GABA-Glutamine Cycle. **23rd Congress on Thermal Science and Technology.**
31. Golcuk M., Hacisuleyman A., Erman B., Yildiz A., **Gur M.** (2021). Exploring the binding mechanisms of nanobodies targeting SARS-CoV-2 spike glycoprotein using molecular dynamics simulations. **2021 ACS Fall Meeting.** (Atlanta, GA) (Invited Speaker)
30. Taka, E., Yilmaz, S.Z., Golcuk, M., Kilinc, C., Aktas, U., Yildiz, A., **Gur, M.** (2021). Critical interactions between the SARS-CoV-2 spike glycoprotein and the human ACE2 receptor. **2021 ACS Spring Meeting.** (Invited Speaker)
29. **Gur, M.** (2021). Molecular Dynamics Simulations of Large Biomolecular Systems. **High Performance Computing Technologies in Drug Design Workshop.** (Invited Speaker)
28. Taka, E., Yilmaz, S.Z., Golcuk, M., Kilinc, C., Aktas, U., Yildiz, A., **Gur, M.** (2021). Critical Interactions Between the SARS-CoV-2 Spike Glycoprotein and the Human ACE2 Receptor. **ITU Department of Chemical Engineering 2nd Graduate Symposium**. (Invited Speaker) Istanbul, Turkey
27. **Gur, M.**, Can, S., Lacey, S., Carter, A. P., Yıldız, A. (2019). Modelling Plus-End-Directed Dyneins. **7th International Congress of the Molecular Biology Association of Turkey (MolBiyoKon19).** Istanbul, Turkey
26. **Gur, M.**, Golcuk, M., Gul, A., Erman, B. (2019). Molecular overview of the role of HLA-B51 in Behçet's Disease. **7th International Congress of the Molecular Biology Association of Turkey (MolBiyoKon19).** Istanbul, Turkey
25. **Gur, M.** (2019). Insight into the mechanochemical cycle of cytoplasmic dynein from molecular dynamics simulations. **7th International BAU Drug Design Congress**. (Invited Speaker) Istanbul, Turkey
24. Golcuk, M., Taka, E., Yilmaz, S.Z., **Gur, M**. (2019). Molecular Dynamics Simulations of the Dynein Linker Movement. **The 12th International Symposium on Health Informatics and Bioinformatics**. Izmır, Turkey
23. Can, S., Lacey, S., **Gur, M.**, Carter, A. P., Yildiz, A. (2019). Dynein's directionality is controlled by the angle and length of its stalk. **63rd Annual Meeting of the Biophysical-Society.** Baltimore, MD
22. **Gur, M.**, Can, S., Lacey, S., Carter, A. P., Yildiz, A. (2018). Engineering plus-end directed dyneins. **6th International BAU Drug Design Congress.** Istanbul, Turkey
21. **Gur, M.**, Gul, A., Erman, B. (2018) Dynamic and static differences between conformations of HLA-B51 and HLA-B52: implications for the pathogenic mechanisms of HLA-B51 in Behçet's disease. **6th International BAU Drug Design Congress**. Istanbul, Turkey

20. **Gur, M.**, Golcuk, M., Yilmaz, S. Z., Taka, E. (2018). Thermodynamic First Law Analysis of Proteins. **6th International BAU Drug Design Congress.** Istanbul, Turkey
19. **Gur, M.** Cheng, M. H., Zomot, E., Bahar, I. (2017). Importance of dimerization in facilitating the functional dynamics of neurotransmitter: sodium symporters. **61st Annual Meeting of the Biophysical-Society**. New Orleans, LA
18. **Gur, M.**, Cheng, M. H., Zomot, E., Bahar, I. (2017). Investigation of the effect of dimerization on the functional dynamics of neurotransmitter: sodium symporters. **5th International BAU-Drug Design Congress**. Istanbul, Turkey
17. **Gur, M.**, Zomot, E., Cheng, M. H., Bahar, I. (2015). Insight into the dynamics of LeuT from multiscale simulations. **Gordon Research Conferences (GRC) Mechanism of Membrane Transport**. Lewiston, ME.
16. **Gur, M.**, Zomot, E., Cheng, M. H., Bahar I. (2014). Toward gaining a mechanistic understanding of substrate transport by LeuT. **Gordon research Conferences (GRC) Biopolymers**. Newport, RI.
15. **Gur, M.**, Zomot, E., Bahar, I. (2014). Global motions of proteins observed in micro to milliseconds simulations concur with Anisotropic Network Model predictions. **Membrane Protein Structural Dynamics Consortium's Annual Meeting**. Chicago, IL
14. Das, A., **Gur, M.**, Bahar, I., Roux, B. (2013). A simple coarse-grained model to map the transition pathway between two stable conformations using the anisotropic elastic network model. **57th Annual Meeting of the Biophysical-Society.** Philadelphia, PA
13. **Gur, M.**, Eskici, G. (2013). Computational design of new peptide inhibitors for amyloid beta aggregation in Alzheimer s disease application of a novel methodology. **American Institute of Chemical Engineers (AIChE) Annual Meeting.** San Francisco, CA.
12. **Gur, M.**, Zomot, E., Bahar, I. (2013). Multiscale investigation of biomolecular systems dynamics. **American Institute of Chemical Engineers (AIChE) Annual Meeting.** San Francisco, CA.
11. **Gur, M.**, Gur, M. (2013). Comparing corn drying in fluidized bed dryer and convective tray dryer. **The Sixth International Exergy, Energy and Environment Symposium.** Rize, Turkey
10. **Gur, M.**, Madura, J., Bahar, I. (2013). Global transitions or proteins explored by a multiscale hybrid methodology: application to dopamine transporter. **57th Annual Meeting of the Biophysical-Society**. Philadelphia, PA
9. **Gur, M.**, Madura, J., Bahar, I. (2012). Transition pathways of Dopamine transporters explored by combining molecular dynamics simulations and Monte Carlo sampling of collective modes. **Membrane Protein Structural Dynamics Consortium's Annual Meeting**. Chicago, IL.
8. **Gur, M.**, Madura, J., Bahar, I. (2012). Transition pathways of proteins explored by combining Molecular Dynamics simulations and Monte Carlo sampling of collective modes. **Biophysical Society 56th Annual Meeting**. Philadelphia, PA.
7. Arkun, Z.Y., **Gur, M.** (2011). Protein folding using coarse grained optimal control and Molecular Dynamics. **18th International Federation of Automatic Control (IFAC) World Congress.** Milano, Italy.
6. **Gur, M.**, Bahar, I. (2011). Transition Pathways of Enzymes Explored by Combining the Anisotropic Network Model, Molecular Dynamics Simulations and a Monte Carlo Sampling of Conformational Space. **Albany 2011: Conversation 17**. Albany, NY.
5. **Gur, M.**, Erman, B. (2010). Harmonic fluctuations of two bound peptides. **Gordon Research Conference (GRC) Biopolymers**. Newport, RI.
4. **Gur, M.**, Erman, B. (2010). Coupling between energy and residue position fluctuations in native proteins. **5th International Symposium on Health Informatics and Bioinformatics**. Antalya, Turkey
3. **Gur, M.**, Erman, B. (2009). Statistical thermodynamics and mode analysis of residue fluctuations in native proteins. **Gordon Research Conference (GRC) Computer Aided Drug Design**. Tilton, NH.

2. **Gur, M.**, Erman, B. (2009). Statistical thermodynamics of residue fluctuations in native proteins. **Biophysical Society 53rd Annual Meeting**. Boston, MS.
1. **Gur, M.**, Erman, B. (2008). Determining binding forces between two peptides using the Gaussian Network Model. **XXI Sitges Conference-Statistical Mechanics of Biopyhsics**. Sitges, Spain

CONFERENCE, SYMPOSIA AND MEETING ORGANIZING

2022 **Scientific Organizing Committee Member**, 8th International BAU-Drug Design Congress

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REVIEWER, EDITORIAL, JURY AND SCREENER SERVICES

JOURNAL REVIEWER SERVICES

ACS Omega (Q1, Impact Factor: 4.132)
ACS Infectious Diseases (Q1, Impact Factor: 5.578)
Advanced Theory and Simulations (Q1, Impact Factor: 4.105)
Biophysical Journal (Q1, Impact Factor: 3.699)
Biopolymers (Q3, Impact Factor: 2.240)
Cell Reports (Q1, Impact Factor: 9.995)
Chemical Physics Letters (Q2, Impact Factor: 2.3)
Computational and Structural Biotechnology Journal (Q1, Impact Factor: 6.155)
EMBO (Q1, Impact Factor: 14.012)
Israel Journal of Chemistry (Q1, Impact Factor: 3.357)
Journal of Biomolecular Structure and Dynamics (Q3, Impact Factor: 5.235)
Journal of Chemical Physics (Q1, Impact Factor: 4.304)
Journal of Molecular Graphics and Modelling (Q2, Impact Factor: 2.942)
Journal of Physical Chemistry B (Q1, Impact Factor: 3.466)
PLOS One (Q1, Impact Factor: 3.752)
PLOS Computational Biology (Q1, Impact Factor: 4.779)
Protein Science (Q1, Impact Factor: 6.993)
Scientific Reports (Q1, Impact Factor: 4.996)
Journal of Physical Chemistry Letters (Q1, Impact Factor: 6.888)
Turkish Journal of Biology (Q3, Impact Factor: 3.245)
Turkish Journal of Chemistry (Q3, Impact Factor: 1.151)

EDITORIAL BOARD DUTIES

2023 – Present Editorial Board Member (Review Editor), ***Frontiers in Molecular Biosciences***
2023 – Present Editorial Board Member (Review Editor), ***Frontiers in Biophysics***
2016 – Present Editorial Board Member, ***Journal of Molecular Graphics and Modelling***

GRANT REVIEWS

THE SCIENTIFIC AND TECHNOLOGICAL RESEARCH COUNCIL OF TURKEY (TUBITAK)

2021 Reviewer; TUBITAK; Academic Research Funding Programs Directorate (ARDEB); Health Sciences; 1002 Short-Term R&D Funding Program Panel

2021 Ad Hoc Reviewer; TUBITAK; Department of Science Fellowships and Grant Programs (BIDEB); 2219-International Postdoctoral Research Fellowship Program for Turkish Citizens Panel

2020 Reviewer; TUBITAK; ARDEB; Electrical, Electronics and Informatics; 1001-The Grant Program for Scientific and Technological Research Projects Panel

2020 Reviewer; TUBITAK; ARDEB; 2209-A-Research Project Support Programme for Undergraduate Students Panel

2019 Ad Hoc Reviewer; TUBITAK; Technology and Innovation Grant Programs Directorate (TEYDEB); Machinery, Manufacturing Technologies Group; 1501-Industrial R&D Projects Grant Program Panel

2019 Moderator, TUBITAK; BIDEB; Biomedical Sciences; 2209-A-Research Project Support Programme for Undergraduate Students

2018 Reviewer; TUBITAK; ARDEB; Engineering; 1002 Short-Term R&D Funding Program Panel

2018 Reviewer; TUBITAK; ARDEB; Engineering; 1001-The Grant Program for Scientific and Technological Research Projects Panel

2018 Reviewer; TUBITAK; ARDEB; Engineering; 3501-National Young Researchers Career Development Program

2018 Reviewer; TUBITAK; ARDEB; Basic Sciences; 1001-The Grant Program for Scientific and Technological Research Projects Panel

2016 Ad Hoc Reviewer; TUBITAK 2504-Italian National Research Council (CNR) and Bilateral Cooperation Program Panel **Health Institutes of Turkey (TUSEB)**

2020 Ad Hoc Reviewer; TUSEB; Computational Structural Biology Strategic R&D Project Grant Call Panel

2019 Ad Hoc Reviewer; TUSEB; Systems Biology and Bioinformatics Strategic R&D Project Grant Call Panel

ISTANBUL TECHNICAL UNIVERSITY

2019 – 2021 Reviewer/Commission Member; Istanbul Technical University; Scientific Research Projects (BAP) Grant Call Panels

2018 – Present Reviewer/Committee Member; Istanbul Technical University; Health and Engineering Sciences Human Research Ethics Project Evaluation Panels

PRACE-PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

2020 Ad Hoc Reviewer; Partnership for Advanced Computing in Europe (PRACE); DECI-16 (Distributed European Computing Initiative) Panel

GRADUATE SCHOOL APPLICATION SCREENING JURY DUTIES

2023 – Present Screener, Computational Biomedicine & Biotechnology (CoBB) M.S. Program led by the Department of Computational & Systems Biology, **University of Pittsburgh School of Medicine**

PROFESSIONAL MEMBERSHIPS

2019 Bioinformatics Association (Turkey)

2013 – 2014 Member of American Institute of Chemical Engineers

2009, 2017 Member of Biophysical Society

RESEARCH INTERESTS

Computational Structural Biology, Computational Molecular Biophysics, Computational Molecular Medicine, Mechanical Engineering

Biomolecular Simulations and Statistical Thermodynamics: Molecular dynamics simulations, Elastic network models, Free energy calculations, Methodology development, *In silico* pulling experiments.
Biomolecular Machines and Motors: Dynein, Kinesin, Microtubules, Microtubule associated proteins
Membranes and Membrane Proteins: Neurotransmitter sodium symporters, Lipids
Drug Design: Cell Penetrating Peptides, Behçet's Disease
Cancer Biology: CHK2, MSH2, MSH6, PR65, Molecular Pathalogy
SARS-CoV-2: Spike Protein, ACE2, Nanobodies
Intrinsically disordered proteins: MAP7, TAU, FapC, Neurodegenerative diseases, Amyloid formation
Thermal and Fluid Sciences: Heat exchangers, Microchip cooling systems, Food drying

ADDITIONAL LEADERSHIP AND COMMUNITY ENGAGEMENT

2023-Present	Volunteer Coach for U-10 team, Pittsburgh Dynamo Youth Soccer (a non-profit educational organization)
2016	Judge, Saint Benoît High School (Istanbul) Robotics Competition
2015-2022	Community Outreach Speaker, Various High Schools: Engaged in promoting science education and career awareness among teenagers through frequent (20+) presentations, seminars, and talks.
2013	Category Judge, Pittsburgh Regional Science and Engineering Fair
2008 – 2010	President, Koc University Graduate Student Association
2007 – 2009	Team Member (Linebacker), Koc University American Football Team (Koc Rams)
2005 – 2006	President, Fenerbahçe Sports Club Supporters University Students Association (1907 UNIFEB), Middle East Technical University Branch

EXTERNAL REVIEWS OF PRIMARY CREATIVE WORK

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"Promising project in cancer treatment: Motor proteins", TRT Haber, Yasemin Küçükkaya, 18 April 2022, https://youtu.be/xUFTHLFn5hA

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http://web.archive.org/web/20201027160009/http://global.itu.edu.tr/news/2020/04/08/international-grant-awarded-to-itu-faculty-member-mert-g%C3%BCr-in-fight-against-coronavirus

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"Our Mechanical Engineering Department faculty member Dr. Mert Gür and Computer Engineering Department faculty member Dr. Ilkay Öksüz met online with İTÜ GVO Ekrem Elginkan High School students to talk about our departments and answered questions from students."
https://twitter.com/itu1773/status/1354041395598733312

US AND EUROPEAN WEBSITES

"Understanding The Biomolecular Nanomachines ın Our Cells", PRACE Digest, 2021
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