EK-3

ÖZGEÇMİŞ

1. Adı Soyadı : İsmail EROL
2. Doğum Tarihi : 21.03.1988
3. Unvanı : Doktor
4. Öğrenim Durumu : Doktora Mezunu
5. Çalıştığı Kurum :

Derece	Alan	Üniversite	Yıl
Lisans	Kimya	Yıldız Teknik Üniversitesi	2011
Y. Lisans	Kimya	Yıldız Teknik Üniversitesi	2015
Doktora	Kimya	Gebze Teknik Üniversitesi	2023

5. Akademik Unvanlar
Yardımcı Doçentlik Tarihi :
Doçentlik Tarihi :
Profesörlük Tarihi :

6. Yönetilen Yüksek Lisans ve Doktora Tezleri
6.1. Yüksek Lisans Tezleri
6.2. Doktora Tezleri

7. Yayınlar
7.1. Uluslararası hakemli dergilerde yayınlanan makaleler (SCI,SSCI,Arts and Humanities)

1. Topaloğlu Aksoy, B.; Senocak, A.; **Erol, I.,** Saglam, M.F.; Kandemir, H.; Sengul I.F.; Cosut, B. (2023) " Meso carbazole linked Bis-BODIPYs: Design, synthesis, structures and properties", *Tetrahedron* Volume 147, 30 October 2023, 133666, https://doi.org/10.1016/j.tet.2023.133666.
2. Ozcan, E.; Saglam, M.F.; Kazan, H.H.; **Erol, I.;** Sengul, I.F.; Cosut, B. (2023) "Indolyl imine substituted BODIPY systems; synthesis, photophysical, and biological properties", *Tetrahedron* Volume 137, 12 May 2023, 133367, https://doi.org/10.1016/j.tet.2023.133367.
3. **Erol, I.;** Kotil, S.E.; Fidan, O.; Yetiman, A.E.; Durdagi, S.; Ortakci, F. (2023) "In Silico Analysis of Bacteriocins from Lactic Acid Bacteria Against SARSCoV-2", *Probiotics and Antimicrobial Proteins*, 15, pages 17–29, https://doi.org/10.1007/s12602-021-09879-0.
4. Topaloğlu Aksoy, B.; **Erol, I.;** Kandemir, H.; Saglam, M.F.; Sengul, I.F.; Cosut, B. (2023) "Investigation of spectroscopic properties of mono and Di-styryl indolecontaining BODIPYs", *Inorganica Chimica Acta*, Volume 544, 1 January 2023, 121230, https://doi.org/10.1016/j.ica.2022.121230.
5. **Erol, I.;** Kotil, S.E.; Ortakci, F.; Durdagi, S. (2023) "Exploring the binding capacity of lactic acid bacteria derived bacteriocins against RBD of SARS-CoV-2 Omicron variant by molecular simulations", *Journal of Biomolecular Structure and Dynamics*, https://doi.org/10.1080/07391102.2022.2158934.
6. Selçuk, B.; **Erol, I.;** Durdagi, S.; Adebali, O. (2022) "Evolutionary association of receptor-wide amino acids with G protein–coupling selectivity in aminergic GPCRs", *Life Science Alliance* Volume 5, No. 10, October 2022, https://doi.org/10.26508/lsa.202201439.
7. Durdagi, S.; Dag, C.; Dogan, B.; Yigin, M.; Avsar, T.; Buyukdag, C.; **Erol, I.** et al. (2021) "Near-physiological-temperature serial crystallography reveals conformations of SARS-CoV-2 main protease active site for improved drug repurposing", Structure Volume 29, Issue 12, 2 December 2021, Pages 1382-1396.e6, https://doi.org/10.1016/j.str.2021.07.007.

8. Tanrıverdi Eçik, E.; Özcan, E.; Kazan, H.H.; **Erol, I.;** Şenkuytu, E.; Çoşut B. (2021) "Dual color triads: synthesis, photophysics and applications in live cell imaging", *New Journal of Chemistry* 45, 9984-9994, https://doi.org/10.1039/D1NJ00900A.
9. **Erol, I.;** Cosut, B.; Durdagi, S. (2019) "Toward Understanding the Impact of Dimerization Interfaces in Angiotensin II Type 1 Receptor", *Journal of Chemical Information and Modeling* 59, 10, 4314–4327, https://doi.org/10.1021/acs.jcim.9b00294.
10. Aytac, Z.; Ipek, S.; **Erol, I.;** Durgun, E.; Uyar, T. (2019) "Fast-dissolving electrospun gelatin nanofibers encapsulating ciprofloxacin/cyclodextrin inclusion complex", *Colloids and Surfaces B: Biointerfaces* Volume 178, 1 June 2019, Pages 129-136, https://doi.org/10.1016/j.colsurfb.2019.02.059.
11. Durdagi, S.; **Erol, I.;** Salmas, R.E.; Aksoydan, B.; Kantarcioglu I. (2019) "Oligomerization and cooperativity in GPCRs from the perspective of the angiotensin AT1 and dopamine D2 receptors", *Neuroscience Letters* Volume 700, 1 May 2019, Pages 30-37, https://doi.org/10.1016/j.neulet.2018.04.028.
12. Durdagi, S.; Dogan, B.; **Erol, I.;** Kayık, G.; Aksoydan, B. (2019) "Current status of multiscale simulations on GPCRs", *Current Opinion in Structural Biology* Volume 55, April 2019, Pages 93-103, https://doi.org/10.1016/j.sbi.2019.02.013.
13. Kanan, T.; Kanan, D.; **Erol, I.;** Yazdi, S.; Stein, M.; Durdagi, S. (2019) "Targeting the NF-κB/IκBα complex via fragment-based E-Pharmacophore virtual screening and binary QSAR models", *Journal of Molecular Graphics and Modelling* Volume 86, January 2019, Pages 264-277, https://doi.org/10.1016/j.jmgm.2018.09.014.
14. Durdagi, S.; Aksoydan, B.; **Erol I.** et al., (2018) "Integration of multi-scale molecular modeling approaches with experiments for the in silico guided design and discovery of novel hERG-Neutral antihypertensive oxazalone and imidazolone derivatives and analysis of their potential restrictive effects on cell proliferation", *European Journal of Medicinal Chemistry* Volume 145, 10 February 2018, Pages 273-290, https://doi.org/10.1016/j.ejmech.2017.12.021.
15. Aksoydan, B.; Kantarcioglu, I.; **Erol, I.;** Salmas, R.E.; Durdagi, S. (2018) "Structure-based design of hERG-neutral antihypertensive oxazalone and imidazolone derivatives", *Journal of Molecular Graphics and Modelling* Volume 79, January 2018, Pages 103-117, https://doi.org/10.1016/j.jmgm.2017.10.011.
16. Salmas, R.E.; Stein, M.; Yurtsever, M.; Seeman, P.; **Erol, I.;** Mestanoglu, M.; Durdagi, S. (2017) "The signaling pathway of dopamine D2 receptor (D2R) activation using normal mode analysis (NMA) and the construction of pharmacophore models for D2R", *Journal of Biomolecular Structure and Dynamics* Volume 35, 2017 - Issue 9, 2040-2048, https://doi.org/10.1080/07391102.2016.1206487.
17. Salmas, R.E.; Seeman, P.; Aksoydan, B.; **Erol, I.;** Kantarcioglu, I.; Stein, M.; Yurtsever, M.; Durdagi, S. (2017) "Analysis of the Glutamate Agonist LY404,039 Binding to Nonstatic Dopamine Receptor D2 Dimer Structures and Consensus Docking", *ACS Chemical Neuroscience* 8, 6, 1404–1415, https://doi.org/10.1021/acschemneuro.7b00070.
18. Durdagi, S.; **Erol, I.;** Salmas, R.E.; Patterson, M.; Noskov, S.Y. (2017) "First universal pharmacophore model for hERG1 K+ channel activators: acthER", *Journal of Molecular Graphics and Modelling* Volume 74, June 2017, Pages 153-170, https://doi.org/10.1016/j.jmgm.2017.03.020.
19. **Erol, I.;** Aksoydan, B.; Kantarcioglu, I.; Salmas, R.E.; Durdagi, S. (2017) "Identification of novel serotonin reuptake inhibitors targeting central and allosteric binding sites: A virtual screening and molecular dynamics simulations study", *Journal of Molecular Graphics and Modelling* Volume 74, June 2017, Pages 193-202, https://doi.org/10.1016/j.jmgm.2017.02.001.
20. Kocak, A.; **Erol, I.;** Yildiz, M.; Can, H. (2016) "Computational insights into the protonation states of catalytic dyad in BACE1–acyl guanidine based inhibitor complex", *Journal of Molecular Graphics and Modelling* Volume 70, November 2016, Pages 226-235, https://doi.org/10.1016/j.jmgm.2016.10.013.
21. **Erol, I.;** Cakar, F.; Ocak, H.; Cankurtaran, H.; Cankurtaran, O.; Bilgin-Eran, B.; Karaman, F. (2016) "Thermodynamic and surface characterisation of 4- [4-((S)-citronellyloxy)benzoyloxy]benzoic acid thermotropic liquid crystal", *Liquid Crystals* Volume 43, 2016 - Issue 1, 142-151, https://doi.org/10.1080/02678292.2015.1067334.
22. Mutlu-Yanic, S.; Guzeller, D.; Ocak, H.; Cakar, F.; Erol, I.; Cankurtaran, O.; Bilgin-Eran, B. (2015) "Synthesis, Preparation, and Characterization of Liquid Crystal/Organo-

Montmorillonite Nanocomposites", *Molecular Crystals and Liquid Crystals* Volume 607, 2015 - Issue 1, 23-31, https://doi.org/10.1080/15421406.2014.927550.

7.2. Uluslararası diğer hakemli dergilerde yayınlanan makaleler
7.3. Uluslararası bilimsel toplantılarda sunulan ve bildiri kitabında basılan bildiriler

1. **Erol, I.;** Cosut, B.; Durdagi, S. (2022) "Atomic Details of Angiotensin II Type 1 and Type II Heterodimers" 8th BAU Drug Design Congress, 15-17 Aralık 2022, Istanbul, Türkiye
2. **Erol, I.;** Cosut, B.; Durdagi, S. (2022) "Unended Quest: In the Search of Dimerization Interfaces of AT1R-AT2R Heterodimer" 2.Computer-Aided Drug Design Symposium and Workshop, 11-12 Mayıs 2022, Istanbul, Türkiye
3. Aytac, Z.; Ipek, S.; **Erol, I.;** Durgun, E.; Uyar, T. (2019) "Fast-dissolving electrospun gelatin nanofibers encapsulating ciprofloxacin/cyclodextrin-inclusion complex" 258th American Chemical Society (ACS) National Meeting & Exposition, 24–29 Ağustos 2019, San Diego, California, USA
4. **Erol, I.;** Cosut, B.; Durdagi, S. (2019) "In The Quest of the Most Plausible Dimerization Interface of the AT1R" 7th BAU Drug Design Congress, 19-21 Aralık 2019, Istanbul, Türkiye
5. **Erol, I.;** Cosut, B.; Durdagi, S. (2018) "Dimerization Interfaces of AT1 Receptor" 6th BAU Drug Design Congress, 13–15 Aralık 2018, Istanbul, Türkiye
6. **Erol, I.;** Cosut, B.; Durdagi, S. (2018) "Computational Insights into Angiotensin II Type 1 Receptor Oligoremization" Early Career Scientist Forum on GPCR Signal Transduction (ECSF-GPCR), 11–14 Temmuz 2018, Berlin, Almanya
7. **Erol, I.;** Aksoydan, B.; Kantarcioglu, I.; Durdagi, S. (2017) "Computational Insights into Angiotensin II Type 1 Receptor (AT1R) Dimerization", 5th BAU Drug Design Congress, 19-21 Ekim 2017, Istanbul, Türkiye
8. **Erol, I.;** Aksoydan, B.; Kantarcioglu, I.; Durdagi, S. (2016) "Dual Acting Serotonin Transporter Inhibitor on Central and Allosteric Binding Site: A Computational Study", 4th BAU Drug Design Congress, 13–15 Ekim 2016, Istanbul, Türkiye.
9. Celik, A.; Canim-Ates, S.; Can, H.; Kusku, S.; **Erol, I.** (2014) "Protein engineering of FDHs for cofactor (NAD(P)H) recycling in reactions catalysed by oxidoreductases", European Biotechnology Congress, 13–15 Mayıs 2014, Lecce, Italya.
10. Ipek-Kusku, S.; **Erol, I.;** Can, H.; Celik, A. (2014) "Computational Engineering of Formate Dehydrogenase: From Catalytic Versatility to Coenzyme Specificity", NanoTr10, 17–21 Haziran 2014, Istanbul, Türkiye
11. Aksakal, F.; Ipek-Kusku, S.; **Erol, I.;** Can, H.; Celik, A. (2014) "In Silico Prediction of Coenzyme Binding Modes and Affinities to the Wild Type and Mutated NADP+ Dependent Formate Dehydrogenase" Chemistry Conference for Young Scientists (ChemCYS), 27–28 Şubat 2014, Blankenberge, Belçika
12. **Erol, I.;** Cakar, F.; Ocak, H.; Bilgin-Eran, B.; Cankurtaran, O.; Karaman, F. (2013) "Investigating Thermodynamic Interactions of 4-[4-((S)-Citronellyloxy) Benzoyloxy] Benzoic Acid (SBBA) Liquid Crystal with Some Solvents by Inverse Gas Chromatography." 15th JCF Frühjahrssymposium, 06–08 Mayıs 2013, Humboldt-Universität zu Berlin, Berlin, Almanya

7.4. Yazılan uluslararası kitaplar veya kitaplarda bölümler

1. **Erol, I.;** Aksoydan, B.; Kantarcioglu, I.; Durdagi, S. (2018) "Application of Multiscale Simulation Tools on GPCRs. An Example with Angiotensin II Type 1 Receptor", Methods in Molecular Biology book series (MIMB, volume 1824), Rational Drug Design, 431-448, https://link.springer.com/protocol/10.1007/978-1-4939-8630-9_26.

7.5. Ulusal hakemli dergilerde yayınlanan makaleler
7.6. Ulusal bilimsel toplantılarda sunulan ve bildiri kitabında basılan bildiriler

1. **Erol, I.;** Kocak, A.; Yildiz, M.; Can, H. (2016) "Investigation of the Catalytic Region of the Beta Secretase Enzyme by Theoretical calculations", 1st Chemistry Innovation Days, 7 Nisan 2016, Gebze Technical University, Kocaeli, Türkiye
2. **Erol, I.;** Aksoydan, B.; Kantarcioglu, I.; Salmas, R.E.; Durdagi, S. (2017) "Novel Orthosteric and Allosteric Serotonin Reuptake Inhibitors : A Virtual Screening and Molecular Dynamics

Study", 2nd Chemistry Innovation Days, 7 Nisan 2017, Gebze Technical University, Kocaeli, Türkiye

3. **Erol, I.;** Aksoydan, B.; Kantarcioglu, I.; Salmas, R.E.; Durdagi, S. (2017) 'Calculation of Binding Free Energies of Serotonin Transporter Inhibitors by MM-PBSA Method' I., 3rd Computational Chemistry Congress, 12–14 Ekim 2017, Ankara, Türkiye

7.7. Diğer yayınlar

1. Durdagi, S.; Aksoydan, B.; **Erol, I.;** Kantarcioglu, I. (2021) "Anti-Kanser İlaçların Tasarımı, Geliştirilmesi ve Keşfi", Bölüm 27, KANSER MOLEKÜLER BİYOLOJİSİ, Editör: Prof. Dr. Yusuf Baran, Hipokrat Yayınevi

8. Projeler

1. "Yeni Nesil Anti-Hipertansif Molekül Olarak Yapı-Bazlı Tasarlanan Oksazolon Ve İmidazolon Türevlerin Fizikokimyasal Ve Biyolojik Özelliklerinin Moleküler Modelleme Ve Biyofiziksel Yöntemler İle Araştırılması Ve Hücre Proliferasyonu Üzerine Olası Kısıtlayıcı Etkilerinin Analizi", **Tübitak Proje Asistanı**, Bahçeşehir Üniversitesi, Tıp Fakültesi, Istanbul, Türkiye, Aralık 2015 – Nisan 2018.
2. "NADP+-Bağımlı Format Dehidrojenaz Enziminin Hesaplamalı ve Deneysel Yöntemlerle Moleküler Mühendisliği", **Tübitak Proje Asistanı**, Gebze Yüksek Teknoloji Enstitüsü, Kocaeli, Türkiye, Şubat 2013 – Şubat 2015.
3. "QC/MM Study of Fumarate Reductase from Shewanella frigidimarina", **Misafir Araştırmacı**, University of Bayreuth, Department of Chemistry, Bayreuth, Germany, Nisan 2015 – Eylül 2015.

9. İdari Görevler

10. Bilimsel ve Mesleki Kuruluşlara Üyelikler

11. Ödüller

12. Son iki yılda verdiğiniz lisans ve lisansüstü düzeydeki dersler için aşağıdaki tabloyu doldurunuz.

Akademik Yıl	Dönem	Dersin Adı	Haftalık Saati		Öğrenci Sayısı
			Teorik	Uygulama	
	Güz				
	İlkbahar				
	Güz				
	İlkbahar				

Not: Açılmışsa, yaz döneminde verilen dersler de tabloya ilave edilecektir.