T.C. KİLİS 7 ARALIK ÜNİVERSİTESİ

AKADEMİK ÖZGEÇMİŞ

Öğr. Gör. Dr. İmren BAYIL

Kilis 7 Aralık Üniversitesi | Uluslararası İlişkiler Koordinatörlüğü

Kişisel ve İletişim Bilgileri

Bilgi	Açıklama
Düzenleme tarihi	16.06.2026
Yazışma adresi	Kilis 7 Aralık Üniversitesi, Uluslararası İlişkiler Koordinatörlüğü, Kilis
E-posta	imren.bayil@kilis.edu.tr
Faks	—

Eğitim

Dönem	Eğitim / Derece	Kurum	Alan / Yer
2017 – 2023	Doktora	Gaziantep Üniversitesi	Biyoinformatik ve Bilişimsel Biyoloji
2013 – 2017	Yüksek Lisans	Gaziantep Üniversitesi	Kimya (Organik Kimya)
2014 - 2015	Dil Eğitimi	Eastbourne School of English	İngiltere
2009 – 2013	Lisans	Ege Üniversitesi	Kimya (İngilizce)

Akademik ve Mesleki Deneyim

Görev Dönemi	Unvan	Üniversite	Bölüm
2026 – Devam	Öğr. Gör. Dr.	Kilis 7 Aralık Üniversitesi	Uluslararası İlişkiler Koordinatörlüğü
2018 – 2023	YÖK 100/2000 Bursiyer Araştırmacı	Gaziantep Üniversitesi	Biyoinformatik ve Bilişimsel Biyoloji

Yayın ve Atıf Göstergeleri

Toplam atıf	h-endeksi	i10-endeksi
628	13	18

Proje Deneyimi

Başvuru notu: TÜBİTAK 2219 Yurt Dışı Doktora Sonrası Araştırma Burs Programı'na 2025 yılında başvurulmuş; proje başlığı: 'Hibrit Perovskitlerde Eş Zamanlı Anahtarlanabilir Kiral-Polar Katyonların Kuantum-Kimya Tabanlı Tasarımı'. Şekil yönünden değerlendirmeye alınmamıştır.

Diğer Akademik Faaliyetler

Editörlük: Journal of Drug Design and Medicinal Chemistry (Editör Kurulu Üyesi, Temmuz 2024 – devam ediyor)

Hakem Kayıtları

1. Novel Drug Design Approaches for the Inhibition of Zika Virus Capsid and Envelope Proteins with Flavonoid-Based Biochemical Compounds.
   PLOS ONE | 2023-12-08
2. Computer-aided aptamer selection for fabrication of electrochemical sensor to detect AFB1.
   Journal of Biomolecular Structure and Dynamics | 2023-12-07
3. A Network Pharmacological Approach for the Identification of Potential Therapeutic Targets of Brahmi Nei - A Complex Traditional Siddha Formulation.
   Journal of Biomolecular Structure and Dynamics | 2023-12-11
4. Guideline-Directed Medical Therapy induced nephrotoxicity in HFrEF patients: an insight into its mechanism.
   Journal of Biomolecular Structure and Dynamics | 2023-12-10
5. Multitargeted docking-based MM/GBSA, QM-DFT, Interaction Fingerprints and Multiscale MD Simulation Delineated Mitoxantrone 2HCl's adroit activity against replication and maintenance proteins of cervical cancer.
   Journal of Biomolecular Structure and Dynamics | 2023-10-28
6. Unraveling biological disparities in configurational isomers of pyrazolyl-dihydrofurans using in vitro, DFT and in silico approach.
   Journal of Biomolecular Structure and Dynamics | 2024-01-17
7. Theoretical investigations of some isolated flavonoids from Calophyllum flavoramulum as potential antioxidant agents and inhibitors of AGEs.
   Journal of Biomolecular Structure and Dynamics | 2024-02-15
8. Mitoxantrone 2HCl's Adroit Activity Against Cervical Cancer Replication and Maintenance Proteins: A Multitargeted Approach.
   Journal of Biomolecular Structure and Dynamics | 2023-10-28

Bilimsel Yayınlar

Yayınlar tek listede, en güncel çalışmadan başlanarak sıralanmıştır. DOI bağlantıları tıklanabilir biçimde verilmiştir.

1. Tayyeb J.Z., et al., **Bayıl I.** Structure-based drug design of sanguinarine derivatives targeting Babesia microti lactate dehydrogenase through computational approaches. Journal of Molecular Graphics and Modelling, 109324, 2026. https://doi.org/10.1016/j.jmgm.2026.109324
2. Ashraf R., Khalid Z., Qin Q.P., Iqbal M.A., Taskin-Tok T., **Bayıl I.**, Quah C.K., Daud N.A.M., Alqahtany F.Z., Amin M.A., El-Bahy S.M. Synthesis of N-heterocyclic carbene-selenium complexes modulating apoptosis and autophagy in cancer cells: Probing the interactions with biomolecules and enzymes. Bioorganic Chemistry, 160, 108435, 2025. https://doi.org/10.1016/j.bioorg.2025.108435
3. Orujova N.S., Abbasov V.M., Jafarova R.A., Mammadov A.M., **Bayıl I.**, Muradova S.A., Djadi N., Alqahtani T., Al-Dies A.M., Zerihun Y.A., Guendouzi A., Zaki M.E.A. In vitro, in silico, and DFT evaluation of antimicrobial imidazole derivatives with insights into mechanism of action. Scientific Reports, 15(1), 37723, 2025. https://doi.org/10.1038/s41598-025-24847-2
4. Tayyeb J.Z., et al., **Bayıl I.** Immunoinformatic strategy for developing multi-epitope subunit vaccine against Helicobacter pylori. PLoS ONE, 2025. https://doi.org/10.1371/journal.pone.0318750
5. Tayyeb J.Z., **Bayıl I.**, Alqashtani T., et al. Identification of therapeutic compounds targeting phosphatidylinositol 3-kinase (PI3K) through molecular docking, dynamics simulation, and DFT calculations. Computational Biology and Chemistry, 118, 108433, 2025. https://doi.org/10.1016/j.compbiolchem.2025.108433
6. Islam M.R., Tayyeb J.Z., Al-Mhyawi S.R., Paul H.K., **Bayıl I.**, et al. Assessment of Annona muricata phytochemicals as 17β-HSD1 inhibitors through molecular docking, dynamics simulation, DFT, and ADMET analyses. Journal of Cellular and Molecular Medicine, 2025. https://doi.org/10.1111/jcmm.70904
7. Tayyeb J.Z., da Silva M.K., Al-Mutairi A.A., Alharbi H.M., Khojah A.A., **Bayıl I.**, Alzahrani A.Y.A., Tóth Z., Oliveira J.I.N., Zaki M.E.A. Evaluation of potential inhibitors of Zika Virus Envelope Protein through molecular docking and dynamics simulation analyses. Virus Research, 361, 199630, 2025. https://doi.org/10.1016/j.virusres.2025.199630
8. Orujova N.S., **Bayıl I.**, et al. (2025). Microwave-Assisted Synthesis and Thermal Properties of 2,4,5-Triphenyl-1-(4-(Phenyldiazenyl)Phenyl)-1H-Imidazole. Processes of Petrochemistry and Oil Refining (PPOR). https://doi.org/10.62972/1726-4685.2025.3.750
9. Ja'afaru S.C., Uzairu A., Hossain S., Ullah M.H., Sallau M.S., Ndukwe G.I., Ibrahim M.T., **Bayıl I.**, Moin A.T. Computer-aided discovery of novel SmDHODH inhibitors for schistosomiasis therapy: Ligand-based drug design, molecular docking, molecular dynamic simulations, drug-likeness, and ADMET studies. PLoS Neglected Tropical Diseases, 18(9), e0012453, 2024. https://doi.org/10.1371/journal.pntd.0012453
10. Akash S., Islam M.R., Bhuiyan A.A., Islam M.N., **Bayıl I.**, Saleem R.M., Albadrani G.M., Al-Ghadi M.Q., Abdel-Daim M.M. In silico evaluation of anti-colorectal cancer inhibitors by Resveratrol derivatives targeting Armadillo repeats domain of APC: molecular docking and molecular dynamics simulation. Frontiers in Oncology, 14, 1360745, 2024. https://doi.org/10.3389/fonc.2024.1360745
11. Akash S., Shanto S.K.H.I., Islam M.R., **Bayıl I.**, Afolabi S.O., Guendouzi A., Abdellattif M.H., Zaki M.E.A. Discovery of novel MLK4 inhibitors against colorectal cancer through computational approaches. Computers in Biology and Medicine, 182, 109136, 2024. https://doi.org/10.1016/j.compbiomed.2024.109136
12. Tayyeb J.Z., Mondal S., Rahman M.A., Kumar S., **Bayıl I.**, Akash S., Hossain M.S., Alqahtani T., Zaki M.E.A., Oliveira J.I.N. Identification of Helicobacter pylori-carcinogenic TNF-alpha-inducing protein inhibitors via daidzein derivatives through computational approaches. Journal of Cellular and Molecular Medicine, 28(9), 2024. https://doi.org/10.1111/jcmm.18358
13. Islam M.R., Tayyeb J.Z., Paul H.K., Islam M.N., Oduselu G.O., **Bayıl I.**, Abdellattif M.H., Al-Ahmary K.M., Al-Mhyawi S.R., Zaki M.E.A. In silico analysis of potential inhibitors for breast cancer targeting 17beta-hydroxysteroid dehydrogenase type 1 (17beta-HSD1) catalyses. Journal of Cellular and Molecular Medicine, 28(15), 2024. https://doi.org/10.1111/jcmm.18584
14. Musa M.S., Islam M.T., Billah W., Hossain M.S., Rahat M.S.S., **Bayıl I.**, et al. Structure-based virtual screening of Trachyspermum ammi metabolites targeting acetylcholinesterase for Alzheimer's disease treatment. PLoS ONE, 19(12), e0311401, 2024. https://doi.org/10.1371/journal.pone.0311401
15. Baba A.M., Shah A.A., **Bayıl I.**, Nayak S., Shyanti R.K., Nissa N., Muzaffar M., Hajam M.A., Akhtar R., Malla B.A., Akhtar S., Singh R.P., Dar N.A. Polydatin inhibits histone deacetylase 1 and shows an anti-angiogenic action in head and neck squamous cell carcinoma. Medical Oncology, 41(11), 2024. https://doi.org/10.1007/s12032-024-02490-7

16. **Bayıl I.**, Hossain M.S., Tamanna S., Uddin M.J., Ahamed F.M., Jardan Y.A.B., Bourhia M. Aptamer biosensor design for the detection of endocrine-disrupting chemicals small organic molecules using novel bioinformatics methods. Journal of Molecular Graphics and Modelling, 108785, 2024.
https://doi.org/10.1016/j.jmgm.2024.108785

17. Islam M.R., Sharma S., Arafat S.Y., Bairagi R.D., Tayyeb J.Z., **Bayıl I.**, et al. Identification of new inhibitors for the avian H1N1 virus through molecular docking and dynamic simulation approaches. Journal of the Indian Chemical Society, 101274, 2024.
https://doi.org/10.1016/j.jics.2024.101274

18. Ja'afaru S.C., Uzairu A., **Bayıl I.**, Sallau M.S., Ndukwe G.I., Ibrahim M.T., Moin A.T., Mollah A.K.M.M., Absar N. Unveiling potent inhibitors for schistosomiasis through ligand-based drug design, molecular docking, molecular dynamics simulations and pharmacokinetics predictions. PLoS ONE, 19(6), e0302390, 2024.
https://doi.org/10.1371/journal.pone.0302390

19. Abdullahi S.H., Moin A.T., Uzairu A., Umar A.B., Ibrahim M.T., Usman M.T., Nawal N., **Bayıl I.**, Zubair T. (2024). Molecular docking studies of some benzoxazole and benzothiazole derivatives as VEGFR-2 target inhibitors: In silico design, MD simulation, pharmacokinetics and DFT studies. Intelligent Pharmacy, 2(2), 232-250.
https://doi.org/10.1016/j.ipha.2023.11.010

20. Akash S., **Bayıl I.**, Hossain M.S., Islam M.R., Hosen M.E., Mekonnen A.B., Nafidi H., Jardan Y.A.B., Bourhia M., Emran T.B. Novel computational and drug design strategies for inhibition of human papillomavirus-associated cervical cancer and DNA polymerase theta receptor by Apigenin derivatives. Scientific Reports, 13(1), 2023.
https://doi.org/10.1038/s41598-023-43175-x

21. Akash S., Abdelkrim G., **Bayıl I.**, Hosen M.E., Mukerjee N., Shater A.F., Saleh F.M., Albadrani G.M., Al-Ghadi M.Q., Abdel-Daim M.M., Tok T.T. Antimalarial drug discovery against malaria parasites through haplopine modification: an advanced computational approach. Journal of Cellular and Molecular Medicine, 27(20), 3168-3188, 2023.
https://doi.org/10.1111/jcmm.17940

22. Akash S., Aovi F.I., Azad M.A.K., Kumer A., Islam M.R., Mukerjee N., Rahman M.M., **Bayıl I.**, Rashid S., Sharma R. A drug design strategy based on molecular docking and molecular dynamics simulations applied to development of inhibitor against triple-negative breast cancer by Scutellarein derivatives. PLoS ONE, 18(10), e0283271, 2023.
https://doi.org/10.1371/journal.pone.0283271

23. Akash S., **Bayıl I.**, Rahman M.A., Mukerjee N., Maitra S., Islam M.R., Rajkhowa S., Ghosh A., Al-Hussain S.A., Zaki M.E.A., Jaiswal V., Sah S., Barboza J.J., Sah R. Target specific inhibition of West Nile virus envelope glycoprotein and methyltransferase using phytocompounds: an in silico strategy leveraging molecular docking and dynamics simulation. Frontiers in Microbiology, 14, 1189786, 2023.
https://doi.org/10.3389/fmicb.2023.1189786

24. Garkusha N.A., Anikeeva O.P., **Bayıl I.**, Taskin-Tok T., Safin D.A. DFT, ADMET, molecular docking and molecular dynamics studies of pyridoxal. Journal of the Indian Chemical Society, 100(3), 100926, 2023.
https://doi.org/10.1016/j.jics.2023.100926

25. Akash S., Hosen M.E., Mahmood S., Supti S.J., Kumer A., Sultana S., Jannat S., **Bayıl I.**, Nafidi H., Jardan Y.A.B., Mekonnen A.B., Bourhia M. Anti-parasitic drug discovery against Babesia microti by natural compounds: an extensive computational drug design approach. Frontiers in Cellular and Infection Microbiology, 13, 1222913, 2023.
https://doi.org/10.3389/fcimb.2023.1222913

26. Akash S., **Bayıl I.**, Mahmood S., Mukerjee N., Mili T.A., Dhama K., Rahman M.A., Maitra S., Mohany M., Al-Rejaie S.S., Ali N., Semwal P., Sharma R. Mechanistic inhibition of gastric cancer-associated bacteria Helicobacter pylori by selected phytocompounds: A new cutting-edge computational approach. Heliyon, 9(10), e20670, 2023.
https://doi.org/10.1016/j.heliyon.2023.e20670

27. Kaya G., Noma S.A.A., Celepci D.B., **Bayıl İ.**, Taskin-Tok T., Gök Y., Ateş B., Aktaş A., Aygün M., Tezcan B. Design, synthesis, spectroscopic characterizations, single crystal X-ray analysis, in vitro xanthine oxidase and acetylcholinesterase inhibitory evaluation as well as in silico evaluation of selenium-based N-heterocyclic carbene compounds. Journal of Biomolecular Structure and Dynamics, 41(21), 11728-11747, 2023.
https://doi.org/10.1080/07391102.2022.2163696

28. Akash S., Mahmood S., Ahamed R., **Bayıl I.**, Bairagi R.D., Islam M.R., Hosen M., De Lima Menezes G., Almaary K.S., Nafidi H., Bourhia M., Ouahmane L. Novel computational and drug design strategies for the inhibition of human T-cell leukemia virus 1-associated lymphoma by Astilbin derivatives. Journal of Biomolecular Structure and Dynamics, 1-16, 2023.
https://doi.org/10.1080/07391102.2023.2294376

Diğer Bilimsel Aktiviteler

1. **İmren BAYIL**. "The Use of Artificial Intelligence in International Relations". 18th International Istanbul Scientific Research Congress, 28-30 Aralık 2025, İstanbul, Türkiye. Sözlü sunum.
2. **İmren BAYIL**. Kimya Eğitiminde Hesaplamalı Yaklaşımların ve Dijital Araçların Etkililiği: Moleküler Modelleme ve Simülasyon Temelli Bir Öğretim Uygulaması. EDUCongress2025-International Education Congress, 2025, Antalya, Türkiye.
3. **İmren BAYIL**, Tuğba TAŞKIN TOK, Gizem TATAR. Detection of Endocrine Disrupting Chemicals with Three-Dimensional DNA Aptamer-Based Biosensors. 3. International Eurasian Multidisciplinary Studies Congress, 4-7 Nisan 2019, Gaziantep Üniversitesi, Türkiye. Sözlü sunum.
4. **İmren BAYIL**, Tuğba TAŞKIN TOK. Modeling of MIL-101 and UMCM-1 Molecules as Biocompatible Metal-Organic Structures and Their Role in Drug Delivery. 4th Pharmaceutical Chemistry Congress, 2016, Kuşadası/İzmir.
5. Seher BAYRAKTAR, **İmren BAYIL**, Tuğba TAŞKIN TOK. Screening of Marine Natural Products Similarity-Based Compounds Against Cancer and Computational Drug Discovery. 9th International Congress of Applied Sciences, 2023.

Sertifikalar ve Mesleki Eğitimler

Yıl	Eğitim / Sertifika	Kurum
2020	Hesaplamalı İlaç Tasarımı	Insight Bio-IT Solutions
2020	Industrial Training in Molecular Modeling and Dynamics	RASA LifeScience Informatics
2020	Docking, QSAR and Molecular Dynamics	Ramaiah Institute of Technology
2019	Python Eğitimi	Mustafa Özgül Yaz Okulu Kursu, Bolu
2018	Biyofizik Yaz Okulu Protein Yapısı ve Etkileşimi	Boğaziçi Üniversitesi, İstanbul
2018	Nanomaterial ve Tıpta Kullanımları	Sanko Üniversitesi, Gaziantep
2016	Pedagojik Formasyon Eğitimi	Gaziantep Üniversitesi
2012	Kalite Kontrol Eğitimi	Kimyagerler Derneği