Asst. Prof. Berna Doğan

Personal Information

Email: bernadogan@itu.edu.tr
Web: https://avesis.itu.edu.tr/bernadogan

International Researcher IDs
ScholarID: veMv2hAAAAAJ
ORCID: 0000-0002-5650-5177
Publons / Web Of Science ResearcherID: S-8930-2018
ScopusID: 57208274406
Yoksis Researcher ID: 311698

Education Information

Post Doctorate, Bahcesehir University, School Of Medıcıne, Department Of Basıc Medıcal Scıences, Turkey 2018 - 2019
Doctorate, Technische Universitaet München, Faculty of Chemistry, Chemistry, Germany 2012 - 2016
Postgraduate, Bogazici University, Faculty Of Arts And Scıences, Department Of Chemıstry, Turkey 2011 - 2012
Undergraduate, Bogazici University, Faculty Of Arts And Scıences, Department Of Chemıstry, Turkey 2005 - 2011

Foreign Languages

English, C1 Advanced

Dissertations

Doctorate, In silico prediction of dissolution rates of pharmaceutical ingredients: Micro-kinetic model based on spiral dissolution, Technische Universitaet München, Faculty of Chemistry, Chemistry, 2016
Postgraduate, Modeling the solvent effect in free radical polymerization and deamidation of peptides, Bogazici University, Faculty Of Arts And Scıences, Department Of Chemıstry, 2012

Research Areas

Physical Chemistry

Academic Titles / Tasks

Assistant Professor, Istanbul Technical University, Fen-Edebiyat, Kimya, 2023 - Continues
Assistant Professor, Bahcesehir University, School Of Medıcıne, Department Of Basıc Medıcal Scıences, 2019 - 2023

Academic and Administrative Experience

Kimya Bölümü Çift Anadal Koordinatörü, Istanbul Technical University, Fen-Edebiyat, Kimya, 2023 - Continues

Courses

Genel Kimya, Undergraduate, 2022 - 2023

Jury Memberships

Post Graduate, Post Graduate, Bahçeşehir Üniversitesi, September, 2020

Published journal articles indexed by SCI, SSCI, and AHCI

I. **Efficient, rapid, and high-yield synthesis of aryl Schiff base derivatives and their in vitro and in silico inhibition studies of hCA I, hCA II, AChE, and BuChE.**
Özil M., Balaydın H. T., Dogan B., Şentürk M., Durdagi S.
Archiv der Pharmazie, 2024 (SCI-Expanded)

II. **Prediction of HIV-1 protease resistance using genotypic, phenotypic, and molecular information with artificial neural networks**
Tunc H., Doğan B., Kiraz B. N. D., Sarı M., Durdagi S., Kotil S.
PeerJ, vol.11, 2023 (SCI-Expanded)

III. **A novel BH3 mimetic Bcl-2 inhibitor promotes autophagic cell death and reduces in vivo Glioblastoma tumor growth**
Calis S., Dogan B., DURDAĞI S., Celebi A., Yapicier O., KILIÇ T., Turanli E. T., Avsar T.
CELL DEATH DISCOVERY, vol.8, no.1, 2022 (SCI-Expanded)

IV. **Design and synthesis of novel caffeic acid phenethyl ester (CAPE) derivatives and their biological activity studies in glioblastoma multiforme (GBM) cancer cell lines**
Sucu B. O., Koc E. B., Savlug Ipek O., Mirat A., Almas F., Guzel M. A., Doğan B., Uludag D., Karakas N., Durdagi S., et al.
Journal of Molecular Graphics and Modelling, vol.113, 2022 (SCI-Expanded)

V. **Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of SARS-CoV-2: A Combined in silico and in vitro Study**
Durdagi S., Orhan M. D., Aksoydan B., Calis S., Doğan B., Sahin K., Shahraki A., Iyison N. B., Avsar T.
Molecular Informatics, vol.41, no.2, 2022 (SCI-Expanded)

VI. **Near-physiological-temperature serial crystallography reveals conformations of SARS-CoV-2 main protease active site for improved drug repurposing**
DURDAĞI S., Dag C., Dogan B., Yigin M., Avsar T., Buyukdag C., Erol I., Ertem F. B., Calis S., Yildirim G., et al.
STRUCTURE, vol.29, no.12, pp.1382-1403, 2021 (SCI-Expanded)

VII. **Investigation of supramolecular interaction of quercetin withN,N-dimethylamine-functionalizedp-sulfonated calix[4,8]arenes using molecular modeling and theirin vitrocytotoxic response towards selected cancer cells**
Oguz M., Doğan B., Durdagi S., Bhatti A. A., Karakurt S., Yilmaz M.
New Journal of Chemistry, vol.45, no.39, pp.18443-18452, 2021 (SCI-Expanded)

VIII. **Synthesis, molecular docking and molecular dynamics studies of novel tacrine-carbamate derivatives as potent cholinesterase inhibitors**
Ozten O., ZENGİN KURT B., Sonmez F., Doğan B., Durdagi S.
Bioorganic Chemistry, vol.115, 2021 (SCI-Expanded)

IX. **Structural and Functional Characterization of Allatostatin Receptor Type-C of Thaumetopoea pityocampa, a Potential Target for Next-Generation Pest Control Agents**
Shahraki A., Işbilir A., Doğan B., Lohse M. J., Durdagi S., Birgul-Iyison N.
Journal of Chemical Information and Modeling, vol.61, no.2, pp.715-728, 2021 (SCI-Expanded)

X. **An Integrated in silico Approach and in vitro Study for the Discovery of Small-Molecule USP7 Inhibitors as Potential Cancer Therapies**

Kanan D., Kanan T., Doğan B., Orhan M. D., Avsar T., Durdagi S.
ChemMedChem, vol.16, no.3, pp.555-567, 2021 (SCI-Expanded)

XI. **Drug Re-positioning Studies for Novel HIV-1 Inhibitors Using Binary QSAR Models and Multi-target-driven In Silico Studies**
Doğan B., Durdagi S.
Molecular Informatics, vol.40, no.2, 2021 (SCI-Expanded)

XII. **Formation of the inclusion complex of water soluble fluorescent calix[4]arene and naringenin: solubility, cytotoxic effect and molecular modeling studies**
Oguz M., Bhatti A. A., Doğan B., Karakurt S., Durdagi S., Yilmaz M.
Journal of Biomolecular Structure and Dynamics, vol.38, no.13, pp.3801-3813, 2020 (SCI-Expanded)

XIII. **Integrating Ligand and Target-Driven Based Virtual Screening Approaches With in vitro Human Cell Line Models and Time-Resolved Fluorescence Resonance Energy Transfer Assay to Identify Novel Hit Compounds Against BCL-2**
Tutumlu G., Dogan B., Avsar T., Orhan M. D., Calis S., DURDAĞI S.
FRONTIERS IN CHEMISTRY, vol.8, 2020 (SCI-Expanded)

XIV. **Synthesis, biological activity and multiscale molecular modeling studies of bis-coumarins as selective carbonic anhydrase IX and XII inhibitors with effective cytotoxicity against hepatocellular carcinoma**
ZENGİN KURT B., DAĞ A., Doğan B., Durdagi S., Angeli A., Nocentini A., Supuran C. T., Sonmez F.
Bioorganic Chemistry, vol.87, pp.838-850, 2019 (SCI-Expanded)

XV. **Current status of multiscale simulations on GPCRs**
Durdagi S., Doğan B., Erol I., Kayık G., Aksoydan B.
Current Opinion in Structural Biology, vol.55, pp.93-103, 2019 (SCI-Expanded)

XVI. **In silico dissolution rates of pharmaceutical ingredients**
Doğan B., Schneider J., Reuter K.
Chemical Physics Letters, vol.662, pp.52-55, 2016 (SCI-Expanded)

XVII. **Free radical polymerization of ethyl methacrylate and ethyl α-hydroxy methacrylate: A computational approach to the propagation kinetics**
Doğan B., Catak S., Van Speybroeck V., Waroquier M., Aviyente V.
Polymer, vol.53, no.15, pp.3211-3219, 2012 (SCI-Expanded)

Supported Projects

Doğan B., Project Supported by Higher Education Institutions, CCR5 reseptörünün yapısal çeşitliliğinin moleküler dinamik MD çalışmaları ile incelenmesi, 2023 - Continues
Doğan B., Durdağı S., Özönder Ş., Avşar T., TUBITAK Project, RNA metilasyon mekanizmasında görevli enzimleri hedef alan moleküllerin moleküler kenetleme,moleküler dinamik ve aktif makine öğrenmesi çalışmaları ile keşfedilmesi, 2024 - 2026
Doğan B., Project Supported by Higher Education Institutions, Makine öğrenmesi yöntemleri kullanarak HDAC izoformları için seçici molekülleri keşfedilmesi, 2023 - 2023
Doğan B., Project Supported by Higher Education Institutions, HDAC6 seçici inhibitörlerin derin makine öğrenmesi yöntemleri ile keşfedilmesi, 2021 - 2023
Doğan B., Durdağı S., Avşar T., Dinç B., Turkey Institutes of Health Administration Project, Etkinligi Kanıtlanmıs, Yeni Öncü BCL-2 Inhibitörlerinin in Siliko Optimizasyon, Sentez, in Vitro ve in Vivo Hayvan Model Çalısmaları, 2020 - 2023
Durdağı S., Doğan B., TUBITAK Project, HIV-1 Yüzey Glikoprotein GP41/GP120 kompleksinin İnsan T-hücre Zarında Bulunan CD4 Reseptörü ve CXCR4/CCR5 koreseptörleri ile Etkileşim Mekanizmasının Çok Boyutlu Moleküler Modelleme ve Uzun Moleküler Dinamik (MD) Simülasyonlar ile İncelenmesi, 2018 - 2019

Activities in Scientific Journals

FRONTIERS IN MOLECULAR BIOSCIENCES, Committee Member, 2023 - Continues
Journal of Drug Design and Medicinal Chemistry, Committee Member, 2022 - Continues

Memberships / Tasks in Scientific Organizations

Turkish Chemical Society, Principal Member, 2023 - Continues, Turkey
The Organization for Women in Science for the Developing World (OWSD) , Member, 2019 - Continues, Italy
Türk Biyofizik Derneği, Member, 2019 - Continues, Turkey
Deutsche Physikalische Gesellschaft e.V, Member, 2013 - 2015, Germany

Scientific Refereeing

PEERJ, Journal Indexed in SCI-E, June 2022
Journal of Microbiology, Biotechnology and Food Sciences, SCI Journal, May 2022
European Journal of Biology, Journal Indexed in SCI-E, December 2021
THERANOSTICS, Journal Indexed in SCI-E, October 2021

Congress and Symposium Activities

Computer Aided Drug Design, Attendee, Vermont, United States Of America, 2023
Visegrad symposium on biomolecular interactions, Invited Speaker, Sopron, Hungary, 2023
Computer Aided Drug Design, Attendee, Vermont, United States Of America, 2019

Scholarships

Yurt İçi Doktora Sonrası Araştırma Burs Programı, TUBITAK, 2018 - 2019
Erasmus Staj Hareketliği, YOK, 2011 - 2011