

1. Adı ve Soyadı: Serdar DURDAĞI

2. Doğum Tarihi: 10/05/1978

3. Unvanı: Prof. Dr.

4. Öğrenim Durumu

Derece	Alan	Üniversite	Yıl
Lisans	Kimya	Hacettepe Üniversitesi	2001
Y. Lisans	Hesaplamalı Kimya	Bilkent Üniversitesi	2004
Doktora	Hesapsal Biyofizik ve Farmasötik Kimya	Freie Universität (FU) Berlin	2009

5. Akademik Ünvanlar

Yardımcı Doçentlik Tarihi: 22.10.2012

Doçentlik Tarihi: 17.05.2013

Profesörlük Tarihi: 01.10.2018

6. Yönetilen Yüksek Lisans ve Doktora Tezleri

6.1. Yüksek Lisans Tezleri

1. EHSAN SAYYAH (2023) Novel resistance-free ret tyrosine kinase inhibitor discovery through dynamic structure-based pharmacophore and qsar modeling and virtual screening of ultra large ligand libraries
2. SAFA HADDAD (2023) Developing novel hERG blocker models using heteroatom type and numbers from extensive ligand libraries
3. EZGİ SAMBUR (2023) Virtual screening of large-scale small molecule libraries against bruton tyrosine kinase effective in chronic lymphocytic leukaemia
4. HANEEN AMMURI (2022) Identification of Novel PARP1 Inhibitors based on Structural Similarities of FDA Approved Drugs.
5. İLAYDA TOLU (2022) In Silico Screening of the FDA and Peptidomimetics and Designing New Peptides against AXL-GAS6 Target
6. NTSOAKI BAITHEDI MOTAPANYANE (2022) Applications of Molecular Modelling Approaches for the Identification of Novel SARS-CoV-2 RDRP Inhibitors
7. ZEYAD TAREQ JASIM ALABDULRAHEEM (2022) Ab initio and Comparative 3D Modeling of FAM222A and Target-Driven-Based Virtual Screening for the Identification of Novel Therapeutics
8. MD KAMRUL HASAN (2021) Molecular Mechanism of AT1R/PARP1 inhibitors interactions using combined molecular modeling approaches and physics-driven virtual identification of novel therapeutics against retinal inflammation
9. AYLAYILDIZ (2020) Determination of the effects of *Chrysophanol* on *pseudomonas aeruginosa* quorum sensing mechanism and biofilm formation via in vitro and in silico methods

10. ASENA HİMMETOĞLU (2020) Machine learning algorithms and combined multi-scale molecular modeling simulations against NADPH oxidase (NOX) enzymes for designing of small molecule therapeutics
11. LALEHAN OKTAY (2020) Integrated ligand- and target-driven-based virtual screening studies for the identification of novel therapeutics against breast cancer
12. ARHUN ALİ BALKAN (2020) Investigation of anti-quorum sensing and anti-biofilm activities on *pseudomonas aeruginosa* of *peltigera* species by lichen and endolichenic fungus specimens in vitro and in silico methods
13. GURBET TUTUMLU (2019) Identification of novel hit molecules against B-cell leukemia/lymphoma-2 (BCL2)
14. VUSLAT ÖYKÜ SAYIN (2019) Structure-based drug design studies for the discovery of novel carbonic anhydrase IX-selective inhibitors
15. IŞIK KANTARCIOĞLU (2017) Discovery of novel AT1 inhibitors using computational methods

6.2. Doktora Tezleri

1. İSMAİL EROL (2023) Investigation of Oligomerization in Membrane Proteins by Computational Methods
2. HIND AL-JANABI (2022) Multiscale drug repurposing study for the treatment of the Alzheimer's disease: A combined in silico and in vitro study
3. BUSECAN AKSOYDAN (2021) An integrated molecular modeling approaches for the novel therapeutics by using cytosolic and membrane-bound target proteins as model systems
3. GÜLŞAH AYDIN (2020) Identification of p53-MDM2 potential inhibitors with virtual screening and multidimensional molecular modeling inhibitors
4. YUSUF SERHAT İŞ (2019) Design of monoamine oxidase enzyme (MAO) inhibitors play important role in the treatment of neurodegenerative diseases using computer aided methods
5. GÜLRU KAYIK (2017) In silico design of hERG non-blocker compounds with retained pharmacological activity using multi-scale molecular modeling applications
6. RAMİN EKHTIARI SALMAS (2015) Multi-scale modeling and investigation of activation mechanisms of G protein-coupled receptors

7. Yayınlar

7.1. Uluslararası hakemli dergilerde yayınlanan makaleler (SCI & SSCI & Arts and Humanities)

1. Sukkar B., Oktay, L., Sahaboglu A., Moayedi A., Zenouri S., Tamer Al-Maghout, Cantó, A., Miranda M., **Durdagi, S.**, Hosseinzadeh Z. Inhibition of altered Orail channel in Müller cells rescues Photoreceptor in degenerated retina. *Glia* 2023 (accepted)

2. Tunc H, Dogan B, Darendeli Kiraz BN, Sari M, **Durdagi S**, Kotil S. Prediction of HIV-1 protease resistance using genotypic, phenotypic, and molecular information with artificial neural networks (2023) *PeerJ*. 2023;11:e14987. doi: 10.7717/peerj.14987.
3. Atalay, N., Akcan, EK., Gul, M., Ayan, E., Destan, E., Ertem, FB., Tokay, N., Cakilkaya, B., Nergiz, Z., Karakadioglu, G., Kepceoglu, A., Yapici, I., Tosun, B., Baldir, N., Yildirim, G., Johnson, JA., Guven, O., Shafiei, A., Arslan, NE., Yilmaz, M., Kulakman, C., Paydos, SS., Cinal, ZS., Sabanoglu, K., Aysegul, P., Yilmaz, A., Canbay, B., Asci, B., Kartal, E.; Tavli, S., Caliseki, M., Goc, G.; Mermer, A., Yesilay, G., Altuntas, S, Tateishi, H., Otsuka, M., Fujita, M., Tekin, S., Ciftci, H., **Durdagi, S.**, Doganay, GD., Karaca, E. Turkoz, BK., Kabasakal, BV., Kati, A., Demirci, H. Cryogenic X-ray crystallographic studies of biomacromolecules at Turkish Light Source "Turkish DeLight" (2023) *Turk. Journal of Biology* 47(1), pp. 1-13.
4. Calis, S., Dogan, B., **Durdagi, S.**, Celebi, A., Yapicier, O., Kilic, T., Turanli, E.T., Avsar, T. A novel BH3 mimetic Bcl-2 inhibitor promotes autophagic cell death and reduces in vivo Glioblastoma tumor growth (2022) *Cell Death Discovery* 8(1), p.433.
5. Erol, I., Kotil, S. E., Ortakci, F., **Durdagi, S.** Exploring the binding capacity of lactic acid bacteria derived bacteriocins against RBD of SARS-CoV-2 Omicron variant by molecular simulations (2022) *Journal of Biomolecular Structure and Dynamics* 1-11. DOI: 10.1080/07391102.2022.2158934
6. Doğan, N., Yavuz, S.Ç., Sahin, K., Orhan, M.D., Kekeçmuhammed, H., Calis, S., Küp, F.Ö., Avsar, T., Akkoc, S., Tapera, M., Sahin, O., Kilic, T., **Durdagi, S.**, Saripinar, E. Synthesis, Characterization, Biological Activity and Molecular Modeling Studies of Novel Aminoguanidine Derivatives (2022) *ChemistrySelect* 7(45), p.e202202819.
7. Tapera, M., Kekeçmuhammed, H., Sahin, K., Krishna, V.S., Lherbet, C., Homberset, H., Chebaiki, M., Tønjum, T., Mourey, L., Zorlu, Y., **Durdagi, S.** Synthesis, characterization, anti-tuberculosis activity and molecular modeling studies of thiourea derivatives bearing aminoguanidine moiety (2022) *Journal of Molecular Structure* 1270, p.133899.
8. Aksoydan, B., **Durdagi, S.** Virtual drug repurposing study for the CGRPR identifies pentagastrin and leuprorelin as putative candidates (2022) *Journal of Molecular Graphics and Modelling* 116, pp. 108254.
9. Onder, F.C., Siyah, P., **Durdagi, S.**, Ay, M., Ozpolat, B. Novel etodolac derivatives as eukaryotic elongation factor 2 kinase (eEF2K) inhibitors for targeted cancer therapy (2022) *RSC Medicinal Chemistry* 13(7), pp.840-849.
10. Onder, F.C., Sahin, K., Senturk, M., **Durdagi, S.**, Ay, M. Identifying highly effective coumarin-based novel cholinesterase inhibitors by in silico and in vitro studies (2022) *Journal of Molecular Graphics and Modelling* 115, p.108210.
11. Sucu, B.O., Koc, E.B., Ipek, O.S., Mirat, A., Almas, F., Guzel, M.A., Dogan, B., Uludag, D., Karakas, N., **Durdagi, S.**, Guzel, M. Design and synthesis of novel caffeic acid phenethyl ester (CAPE) derivatives and their biological activity studies in glioblastoma multiforme (GBM) cancer cell lines (2022) *Journal of Molecular Graphics and Modelling* 113, p.108160.
12. Zaka, M., Mohammed, F., Fareed, A. F., **Durdagi, S.** Development of deep learning based QSAR models for the identification of novel anti-cancer therapeutics against malignant glioma from ultra large libraries (2022). *Biophysical Journal* 121(3), 529a.

13. **Durdagi, S.**, Avsar, T., Orhan, M.D., Serhatli, M., Balcioglu, B.K., Ozturk, H.U., Kayabolen, A., Cetin, Y., Aydinlik, S., Bagci-Onder, T., Tekin, S. The neutralization effect of montelukast on SARS-CoV-2 is shown by multiscale in silico simulations and combined in vitro studies (2022) *Molecular Therapy* 30(2), pp.963-974.
14. Cetin, Y., Aydinlik, S., Gungor, A., Kan, T., Avsar, T., **Durdagi, S.** Review on in silico methods, high-throughput screening techniques, and cell culture based in vitro assays for SARS-CoV-2 (2022) *Current Medicinal Chemistry* 29(38), pp.5925-5948.
15. Mansoor, S., Kayik, G.; **Durdagi, S.**; Sensoy, O. Mechanistic insight into the impact of a bivalent ligand on the structure and dynamics of a GPCR oligomer (2022) *Computational and Structural Biotechnology Journal* 20, pp. 925-936.
16. Aksoydan, B., **Durdagi, S.** Molecular simulations reveal the impact of RAMP1 on ligand binding and dynamics of calcitonin gene-related peptide receptor heterodimer (2022) *Computers in Biology and Medicine* 141 pp. 105130.
17. **Durdagi, S.**, Avsar, T., Orhan, MD., Serhatli, M., Balcioglu, B.K., Ozturk, H.U., Kayabolen, A., Cetin, Y., Aydinlik, S., Bagci-Onder, T., Tekin, S., Demirci, H., Guzel, M., Akdemir, A., Calis, S., Oktay, L., Tolu, I., Butun, Y.E., Erdemoglu, C., Olkan, A., Tokay, N., Isik, S., Ozcan, A., Acar, E., Buyukkilic, S., Yumak, Y. The neutralization effect of Montelukast on SARS-CoV-2 is shown by multiscale in silico simulations and combined in vitro studies (2022) *Molecular Therapy* 30(2), pp.963-974.
18. Balli, OI., Uversky, VN., **Durdagi, S.**, Coskuner-Weber, O. Challenges and limitations in the studies of glycoproteins: A computational chemist's perspective (2022) *Proteins - Structure Function and Bioinformatics* 90(2), pp322-339.
19. Bayrak, C., Yildizhan, G., Kilinc, N., **Durdagi, S.**, Menzek, A. Synthesis and aldose reductase inhibition effects of novel N-benzyl-4-methoxyaniline derivatives (2021) *Chemistry and Biodiversity* 19(1):e202100530.
20. Dogan, K., Erol, E., Orhan, MD., Degirmenci, Z., Kan, T., Gungor, A., Yasa, B. Avsar, T., Cetin, Y., **Durdagi, S.**, Guzel, M. Instant determination of the artemisinin from various *Artemisia annua* L. extracts by LC-ESI-MS/MS and their in-silico modelling and in vitro antiviral activity studies against SARS-CoV-2 (2022) *Phytochemical Analysis*, 33(2), pp303-319.
21. **Durdagi, S.**, Orhan, MD., Aksoydan, B., Calis, S., Dogan, B., Sahin, K., Shahraki, A., Iyison, NB., Avsar, T. Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of SARS-CoV-2: A Combined in silico and in vitro Study (2022) *Molecular Informatics* DOI: 10.1002/minf.202100062
22. Sucu, B.O., Koc, E.B., Savlug, O., Mirat, A., Almas, F., Guzel, M.A., Dogan, B., Uludag, D., Karakas, N., **Durdagi, S.**, Guzel, M. Synthesis of Novel Caffeic Acid Phenethyl Ester (CAPE) Derivatives and Their Biological Activity Studies in Glioblastoma Multiforme (GBM) Cancer Cell Lines (2021) *Journal of Molecular Graphics and Modelling* 113, pp.108160.
23. Guven, O., Gul, M., Ayan, E., Gocenler O., Buyukdag, C., Johnson, J.A., Cakilkaya, B., Usta, G., Ertem, F.B., Tokay, N., Yuksel, B., Botha S. Ketewala, G., Su, Z., Hayes, B., Poitevin, F., Yoon, C.H., Kupitz, C., **Durdagi, S.**, Sierra, R.G., Demirci, H. Case Study of High Throughput Drug Screening and Remote Data Collection for SARS-CoV-2 Main Protease by Using Serial Femtosecond X-ray Crystallography (2021) *Crystals* 11(12), pp.1579.

24. **Durdagi S**, Dağ Ç, Dogan B, Yigin M, Avsar T, Buyukdag C, Erol I, Ertem FB, Calis S, Yildirim G, Orhan MD, Guven O, Aksoydan B, Destan E, Sahin K, Besler SO, Oktay L, Shafiei A, Tolu I, Ayan E, Yuksel B, Peksen AB, Gocenler O, Yucel AD, Can O, Ozabrahamyan S, Olkan A, Erdemoglu E, Aksit F, Tanisali G, Yefanov OM, Barty A, Tolstikova A, Ketawala GK, Botha S, Dao EH, Hayes B, Liang M, Seaberg MH, Hunter MS, Batyuk A, Mariani V, Su Z, Poitevin F, Yoon CH, Kupitz C, Sierra RG, Snell EH, DeMirici H. Near-physiological-temperature serial crystallography reveals conformations of SARS-CoV-2 main protease active site for improved drug repurposing (2021) *Structure* 29(12), pp.1382-1396.e6. doi: 10.1016/j.str.2021.07.007.
25. Oguz, M., Dogan, B., **Durdagi, S.**, Bhatti, AA., Karakurt, S., Yilmaz, M. In vitro Cytotoxic Assay and Numerical Investigation of Inclusion Complex of Calix[4,8]arene and Quercetin (2021) *New Journal of Chemistry* 45, pp18443-18452.
26. Sahin, K., Saripinar, E., **Durdagi, S.** Determination of Bioactive Pharmacophore Groups in Isatin Derivatives with Combined 4D-QSAR and Target-driven Approaches (2021) *SAR and QSAR Environmental Research* DOI: 10.1080/1062936X.2021.1971760.
27. Ozten O, Zengin Kurt B, Sonmez F, Dogan B, **Durdagi S.** Synthesis, molecular docking and molecular dynamics studies of novel tacrine-carbamate derivatives as potent cholinesterase inhibitors (2021) *Bioorg Chem.* 115:105225. doi: 10.1016/j.bioorg.2021.105225.
28. Oktay, L., Erdemoglu, E., Tolu, I., Yumak, Y., Ozcan, A., Acar, E., Buyukkilic, S., Olkan, A., **Durdagi, S.** Binary-QSAR guided virtual screening of FDA approved drugs and compounds in clinical investigation against SARS-CoV-2 main protease (2021) *Turk. J. Biol.* 45, pp459-468.
29. Erol, I., Fidan, O., Yetiman, A., Kotil, E., **Durdagi, S.**, Ortakci, F. In Silico Analysis of Bacteriocins from Lactic Acid Bacteria Against SARS-CoV-2 (2021) *Probiotics and Antimicrobial Proteins* DOI: 10.1007/s12602-021-09879-0.
30. Kanan, T., Kanan, D., Jaffar, I., **Durdagi, S.** Transcription Factor NF- κ B as Target for SARS-CoV-2 Drug Discovery Efforts Using Inflammation-based QSAR Screening Model (2021) *Journal of Molecular Graphics and Modelling* 108, pp107968.
31. Siyah, P., Akgol, S., **Durdagi, S.**, Kocabas, F. Identification of first-in-class plasmodium OTU inhibitors with potent anti-malarial activity (2021) *Biochemical Journal* 478 (18), pp3445–3466.
32. Güngör, T., Ozleyen, A., Yılmaz, Y.B., Siyah, P., Ay, M., **Durdagi, S.**, Tumer, T.B. New nimesulide derivatives with amide/sulfonamide moieties: Selective COX-2 inhibition and antitumor effects (2021) *European Journal of Medicinal Chemistry*, 221, DOI: 10.1016/j.ejmech.2021.113566.
33. Ikram, S., Ahmad, F., Ahmad, J., **Durdagi, S.** Screening of small molecule libraries using combined text mining, ligand- and target-driven based approaches for identification of novel granzyme H inhibitors (2021) *Journal of Molecular Graphics and Modelling*, 105, DOI: 10.1016/j.jmgm.2021.107876
34. Onder, F.C, Kahraman, N., Bellur Atici, E., Cagir, A., Kandemir, H., Tatar, G., Taskin Tok, T., Kara, G., Karliga, B., **Durdagi, S.**, Ay, M., Ozpolat, B. Target-Driven Design of a Coumarinyl Chalcone Scaffold Based Novel EF2 Kinase Inhibitor Suppresses Breast Cancer Growth in Vivo (2021) *ACS Pharmacology and Translational Science*, 4 (2), pp. 926-940.

35. Shahraki, A., İşbilir, A., Dogan, B., Lohse, M.J., **Durdagi, S.**, Birgul-Iyison, N. Structural and Functional Characterization of Allatostatin Receptor Type-C of *Thaumatococcus panyocarpa*, a Potential Target for Next-Generation Pest Control Agents (2021) *Journal of Chemical Information and Modeling*, 61 (2), pp. 715-728.
36. Kanan, D., Kanan, T., Dogan, B., Orhan, M.D., Avsar, T., **Durdagi, S.** An Integrated in silico Approach and in vitro Study for the Discovery of Small-Molecule USP7 Inhibitors as Potential Cancer Therapies (2021) *ChemMedChem*, 16 (3), pp. 555-567.
37. Dogan, B., **Durdagi, S.** Drug Re-positioning Studies for Novel HIV-1 Inhibitors Using Binary QSAR Models and Multi-target-driven In Silico Studies (2021) *Molecular Informatics*, 40 (2), DOI: 10.1002/minf.202000012
38. Akbayrak, I.Y., Caglayan, S.I., **Durdagi, S.**, Kurgan, L., Uversky, V.N., Ulver, B., Dervisoglu, H., Haklidir, M., Hasekioglu, O., Coskuner-Weber, O. Structures of MERS-CoV macro domain in aqueous solution with dynamics: Impacts of parallel tempering simulation techniques and CHARMM36m and AMBER99SB force field parameters (2021) *Proteins: Structure, Function and Bioinformatics*, DOI: 10.1002/prot.26150
39. Sahin, K., Orhan, M.D., Avsar, T., **Durdagi, S.** Hybrid in Silico and TR-FRET-Guided Discovery of Novel BCL-2 Inhibitors (2021) *ACS Pharmacology and Translational Science*, DOI: 10.1021/acspsci.0c00210
40. Sahin, K., **Durdagi, S.** Identifying new piperazine-based PARP1 inhibitors using text mining and integrated molecular modeling approaches (2021) *Journal of Biomolecular Structure and Dynamics*, 39 (2), pp. 681-690.
41. Onder, F.C., **Durdagi, S.**, Kahraman, N., Uslu, T.N., Kandemir, H., Atici, E.B., Ozpolat, B., Ay, M. Novel inhibitors of eukaryotic elongation factor 2 kinase: In silico, synthesis and in vitro studies (2021) *Bioorganic Chemistry*, DOI: 10.1016/j.bioorg.2021.105296
42. Avsar, T., Yigit, B.N., Turan, G., Altunsoy, D., Calis, S., Kurt, B., Kilic, T., Ergun, M.Y., **Durdagi, S.**, Acar, M. Development of imidazolone based angiotensin II receptor type I inhibitor small molecule as a chemotherapeutic agent for cell cycle inhibition (2021) *All Life*, 14(1), pp678-690.
43. Ikram, S., Ahmad, J., Rehman, I.-U., **Durdagi, S.** Potent novel inhibitors against hepatitis C virus NS3 (HCV NS3 GT-3a) protease domain (2020) *Journal of Molecular Graphics and Modelling*, 101, DOI: 10.1016/j.jmglm.2020.107727
44. Ahmad, J., Ikram, S., Hafeez, A.B., **Durdagi, S.** Physics-driven identification of clinically approved and investigation drugs against human neutrophil serine protease 4 (NSP4): A virtual drug repurposing study (2020) *Journal of Molecular Graphics and Modelling*, 101, DOI: 10.1016/j.jmglm.2020.107744
45. Birgul Iyison, N., Sinmaz, M.G., Duan Sahbaz, B., Shahraki, A., Aksoydan, B., **Durdagi, S.** In silico characterization of adipokinetic hormone receptor and screening for pesticide candidates against stick insect, *Carausius morosus* (2020) *Journal of Molecular Graphics and Modelling*, 101, DOI: 10.1016/j.jmglm.2020.107720
46. Turan, R.D., Albayrak, E., Uslu, M., Siyah, P., Alyazici, L.Y., Kalkan, B.M., Aslan, G.S., Yucel, D., Aksoz, M., Tuysuz, E.C., Meric, N., **Durdagi, S.**, Gulbas, Z., Kocabas, F. Development of Small Molecule MEIS Inhibitors that modulate HSC activity (2020) *Scientific Reports*, 10 (1), art. no. 7994, DOI: 10.1038/s41598-020-64888-3

47. Kulabas, S.S., Onder, F.C., Yılmaz, Y.B., Ozleyen, A., **Durdagi, S.**, Sahin, K., Ay, M., Tumer, T.B. In vitro and in silico studies of nitrobenzamide derivatives as potential anti-neuroinflammatory agents (2020) *Journal of Biomolecular Structure and Dynamics*, 38 (15), pp. 4655-4668.
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49. Is, Y.S., Aksoydan, B., Senturk, M., Yurtsever, M., **Durdagi, S.** Integrated Binary QSAR-Driven Virtual Screening and in Vitro Studies for Finding Novel hMAO-B-Selective Inhibitors (2020) *Journal of Chemical Information and Modeling*, 60 (8), pp. 4047-4055.
50. Sahin, K., Zengin Kurt, B., Sonmez, F., **Durdagi, S.** Novel AChE and BChE inhibitors using combined virtual screening, text mining and in vitro binding assays (2020) *Journal of Biomolecular Structure and Dynamics*, 38 (11), pp. 3342-3358.
51. Aydin, G., Paksoy, M.N., Orhan, M.D., Avsar, T., Yurtsever, M., **Durdagi, S.** Proposing novel MDM2 inhibitors: Combined physics-driven high-throughput virtual screening and in vitro studies (2020) *Chemical Biology and Drug Design*, 96 (1), pp. 684-700.
52. Sahaboglu, A., Miranda, M., Canjuga, D., Avci-Adali, M., Savytska, N., Secer, E., Feria-Pliego, J.A., Kayık, G., **Durdagi, S.** Drug repurposing studies of PARP inhibitors as a new therapy for inherited retinal degeneration (2020) *Cellular and Molecular Life Sciences*, 77 (11), pp. 2199-2216.
53. Gunay, B.C., Yurtsever, M., **Durdagi, S.** Elucidation of interaction mechanism of hERG1 potassium channel with scorpion toxins BeKm-1 and BmTx3b (2020) *Journal of Molecular Graphics and Modelling*, 96, DOI: 10.1016/j.jmgm.2019.107504
54. Tutumlu, G., Dogan, B., Avsar, T., Orhan, M.D., Calis, S., **Durdagi, S.** 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 (2020) *Frontiers in Chemistry*, 8, DOI: 10.3389/fchem.2020.00167
55. Comert Onder, F., **Durdagi, S.**, Sahin, K., Ozpolat, B., Ay, M. Design, Synthesis, and Molecular Modeling Studies of Novel Coumarin Carboxamide Derivatives as eEF-2K Inhibitors (2020) *Journal of Chemical Information and Modeling*, 60 (3), pp. 1766-1778.
56. Ikram, S., Ahmad, J., **Durdagi, S.** Screening of FDA approved drugs for finding potential inhibitors against Granzyme B as a potent drug-repurposing target (2020) *Journal of Molecular Graphics and Modelling*, 95, DOI: 10.1016/j.jmgm.2019.107462
57. Zengin Kurt, B., **Durdagi, S.**, Celebi, G., Ekhteiri Salmas, R., Sonmez, F. Synthesis, anticholinesterase activity and molecular modeling studies of novel carvacrol-substituted amide derivatives (2020) *Journal of Biomolecular Structure and Dynamics*, 38 (3), pp. 841-859.
58. Kuskucu, M., Akyildiz, V., Kulmány, Á., Ergün, Y., Zencir, S., Zupko, I., **Durdagi, S.**, Zaka, M., Sahin, K., Orhan, H., Topcu, Z. Structural modification of ellipticine derivatives with alkyl groups of varying length is influential on their effects on human DNA topoisomerase II: a combined experimental and computational study (2020) *Medicinal Chemistry Research*, 29 (2), pp. 189-198.

59. Zaka, M., Abbasi, B.H., **Durdagi, S.** Novel tumor necrosis factor- α (TNF- α) inhibitors from small molecule library screening for their therapeutic activity profiles against rheumatoid arthritis using target-driven approaches and binary QSAR models (2019) *Journal of Biomolecular Structure and Dynamics*, 37 (9), pp. 2464-2476.
60. Kurt, B.Z., Dag, A., Doğan, B., **Durdagi, S.**, Angeli, A., Nocentini, A., Supuran, C.T., Sonmez, F. 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 (2019) *Bioorganic Chemistry*, 87, pp. 838-850.
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63. Ntountaniotis, D., Andreadelis, I., Kellici, T.F., Karageorgos, V., Leonis, G., Christodoulou, E., Kiriakidi, S., Becker-Baldus, J., Stylos, E.K., Chatziathanasiadou, M.V., Chatzigiannis, C.M., Damalas, D.E., Aksoydan, B., Javornik, U., Valsami, G., Glaubitz, C., **Durdagi, S.**, Thomaidis, N.S., Kolocouris, A., Plavec, J., Tzakos, A.G., Liapakis, G., Mavromoustakos, T. Host-Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl- β -cyclodextrin: On the Biological Potency for Angiotensin II Antagonism (2019) *Molecular Pharmaceutics*, 16 (3), pp. 1255-1271.
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63. Salmas vd. *Journal of Enzyme Inhibition and Medicinal Chemistry* (2016), toplam atıf sayısı: 17
64. Guo vd. *PLoS ONE* (2014), toplam atıf sayısı: 17
65. Durdagi vd. *BMC Pharmacology and Toxicology* (2014), toplam atıf sayısı: 17
66. Agelis vd. *Journal of Computer-Aided Molecular Design* (2010), toplam atıf sayısı: 16
67. Tutumlu vd. *Frontiers in Chemistry* (2020), toplam atıf sayısı: 15
68. Durdagi vd. *Turkish Journal of Biology* (2020), toplam atıf sayısı: 15
69. Kellici vd. *Current Medicinal Chemistry* (2016), toplam atıf sayısı: 15
70. Ntountaniotis vd. *Molecular Pharmaceutics* (2019), toplam atıf sayısı: 14
71. Durdagi vd. *European Journal of Medicinal Chemistry* (2018), toplam atıf sayısı: 14
72. Salmas vd. *ACS Chemical Neuroscience* (2017), toplam atıf sayısı: 14
73. Salmas vd. *Biophysical Journal* (2015), toplam atıf sayısı: 14
74. Turan vd. *Scientific Reports* (2020), toplam atıf sayısı: 13
75. Aksoydan vd. *Journal of Molecular Graphics and Modelling* (2018), toplam atıf sayısı: 13
76. Kapou vd. *Journal of Chemical Information and Modeling* (2008), toplam atıf sayısı: 13
77. Durdagi vd. *Structure* (2021), toplam atıf sayısı: 12
78. Ozten vd. *Bioorganic Chemistry* (2021), toplam atıf sayısı: 12
79. Gungor vd. *European Journal of Medicinal Chemistry*, toplam atıf sayısı: 12
80. Oguz vd. *Journal of Biomolecular Structure and Dynamics* (2020), toplam atıf sayısı: 12
81. Sahaboglu vd. *Cellular and Molecular Life Sciences* (2020), toplam atıf sayısı: 12
82. Onder vd. *Journal of Chemical Information and Modeling* (2020), toplam atıf sayısı: 12
83. Zaka vd. *Journal of Biomolecular Structure and Dynamics* (2019), toplam atıf sayısı: 12

84. Durdagi vd. Neuroscience Letter (2019), toplam atıf sayısı: 12
85. Orhan vd. Bioorganic Chemistry (2019), toplam atıf sayısı: 12
86. Salmas vd. Journal of Biomolecular Structure and Dynamics (2017), toplam atıf sayısı: 12
87. Salmas vd. Journal of Biomolecular Structure and Dynamics (2017), toplam atıf sayısı: 12
88. Ekinci vd. Journal of Enzyme Inhibition and Medicinal Chemistry (2013), toplam atıf sayısı: 12
89. Durdagi vd. Bioorganic and Medicinal Chemistry (2008), toplam atıf sayısı: 12
90. Durdagi vd. Molecular Therapy (2022), toplam atıf sayısı: 11
91. Durdagi vd. Current Opinion in Structural Biology (2019), toplam atıf sayısı: 11
92. Talaz vd. Bioorganic and Medicinal Chemistry (2013), toplam atıf sayısı: 11

*10 üzerinde atıf alan makaleler lislenmiştir. Toplam atıf sayısı: 3275, h-endeks: 33

8. Ulusal & Uluslararası Projeler

1. Targeting RNA as an approach for treating retinal disease (RETORNA), EU Horizon Europe (2023-2027), Proje yürütücüsü
2. Molekül Veri Bankalarından Yeni IL-17A İnhibitörü Moleküllerin Belirlenmesi ve Multipl Sklerozda Enflamasyonu Baskılamadaki Etkinliğinin İn in Vitro vitro ve İn in Vivo vivo Yöntemlerle Araştırılması, TÜBİTAK-1001, Araştırmacı, (2023-2025)
3. 18AG020, Ülkemizde ve Dünyada Halk Sağlığını En Fazla Tehdit Eden HIV, HPV ve Influenza Kaynaklı Enfeksiyonlara Karşı Tanı Kitleri, İlaç Formülasyonları ve Aşı Geliştirilmesi, TÜBİTAK 1004, Mükemmeliyet Merkezi Destek Programı, Araştırmacı, (2020-2022)
4. 119N234, Malign Gliomaya Karşı Makine Öğrenmeye Dayalı Yeni Anti Kanser Terapötik Moleküllerin Geliştirilmesi, TÜBİTAK Uluslararası, UPAG (2020-2022), Proje Yürütücüsü
5. Kötü farmakokinetik parametrelere sahip kullanılan ilaçların ve prelinik ve klinik safhalarda çalışılan ilaç adayları küçük moleküllerin in siliko yöntemler ile rehabilite edilerek beyin tümörlerine karşı kullanılması, TÜSEB, Proje Yürütücüsü, (2020-2022)
6. 215S008, Moleküler Modelleme Tabanlı, Kanser Tedavisine Yönelik Protein Kinaz İnhibitörlerin Tasarımı, Sentezi, Denetimli Salım İle In Vitro Ve In Vivo Etkinliklerinin İncelenmesi, TÜBİTAK 1003, Araştırmacı (2016-2021)
7. 215S681, Metilmalonil Koenzim A Mutaz Enziminin Konformasyonel Bozukluğuna Bağlı Olarak Gelişen Metilmalonik Asidemi Hastalığında Farmakolojik Şaperon Uygulaması İle Enzim Aktivitesinin Yeniden Kazandırılması, TÜBİTAK 1001, Araştırmacı (2017-2020)
8. 218S752, Akciğer Kanseri İmmün Kontrol Noktası (Checkpoint) İle Çoğunluğu Algılama Sistemi (QS) Arasındaki Potansiyel İlişkinin Liken Sekonder Metabolitleriyle İnhibisyonunun Araştırılması, TÜBİTAK COST, (2019-2021), Araştırmacı
9. 216S297, Parkinson Hastalığının Tedavisinde Birden Fazla Reseptörü Hedefleyebilen Özgün Terapötik Moleküllerin Geliştirilmesi, TÜBİTAK COST, (2017-2022), Araştırmacı
10. 216S885, Türk Liken Biyokaynakları Kullanılarak Bakteriyel Quorum Sensing İnhibitörü Yeni Antimikrobiyal Bileşenlerin Geliştirilmesi ve Sanayiye Aktarılması,

TÜBİTAK COST, (2017-2019), Araştırmacı

11. Dengue Virüsüne Karşı Yeni Hedeflerin Bilgisayar Destekli İlaç Tasarımı Teknikleri ile Geliştirilmesi; TÜBİTAK 2216 (Uluslararası Araştırmacılar İçin Araştırma Burs Programı). Bahçeşehir Üniversitesi, Tıp Fakültesi (2015-2016) Proje Danışmanı
12. Potasyum iyon kanalı human *ether-a-go-go-related* gene (hERG) için ligand ve yapı bazlı 3 boyutlu atomistik modellerin oluşturulması, bu modellerin validasyon çalışmalarının yapılması ve geliştirilen modellerde ligand/reseptör etkileşimlerinin teorik incelenmesi. (Kanada Sağlık Araştırmaları Enstitüsü-*Canadian Institute of Health Research (CIHR)* Araştırma Fonu (201103MOP-CSA-244888). (2011-2013) Proje Yürütücüsü
13. Nörodejeneratif hastalıklara karşı geliştirilme potansiyeli olan yeni ilaçlar için potent biyoaktif moleküllerin çeşitli ortamlarda yapı ve dinamik özelliklerinin moleküler mekanik ve kuantum mekanik teknikleri ile incelenmesi. Ulusal Yunan Araştırma Kurumu-*National Hellenic Research Foundation (NHRF)*, Avrupa Birliği 6. Çerçeve Marie-Curie Actions Araştırma Fonu (EURODESY-MEST-CT-2005-02057) (2006-2009), Marie Curie Bursiyeri
14. 214S122, Acne Vulgaris Hastalığının Etmenlerinin *Propionibacterium Acnes* Bakterisinin Liken Türlerinden İzole Edilen Sekonder Metabolitler Kullanılarak Biyofilm Oluşturulmasının Engellenmesi, TÜBİTAK COST, (2015-2018), Araştırmacı
15. Potasyum iyon kanallarının *in silico* çalışılması: Modelleme, simülasyon ve yeni algoritmalar geliştirilmesi. TÜBİTAK 2236 (Uluslararası Deneyimli Araştırmacı Dolaşım Destek Programı), (2013-2015) Proje Yürütücüsü
16. 214Z122, Yeni Nesil Anti-Hipertansif Molekül Olarak Yapı-Bazlı Tasarlanan Okşazolon Ve İmidazolon Türevlerin Fizikokimyasal ve Biyolojik Özelliklerinin Moleküler Modelleme ve Biyofiziksel Yöntemler ile Araştırılması ve Hücre Proliferasyonu Üzerine Olası Kısıtlayıcı Etkilerinin Analizi; TÜBİTAK 1001 (Bilimsel ve Teknolojik Araştırma Projelerini Destekleme Programı), (2015-2018) Proje Yürütücüsü

9. İdari Görevler

1. Dekan, Bahçeşehir Üniversitesi Eczacılık Fakültesi (2022-)
2. Temel Tıp Bilimleri Bölüm Başkanı, Bahçeşehir Üniversitesi Tıp Fakültesi, (2019-2022)
3. Dekan Yrd., Bahçeşehir Üniversitesi, Tıp Fakültesi (2014 - 2018)
4. Senato Üyesi, Bahçeşehir Üniversitesi (2019-)
5. Sürekli Mesleki Gelişim Komisyonu, Bahçeşehir Üniversitesi, Tıp Fakültesi (2019-2022)
6. Ölçme Değerlendirme Kurulu Üyesi, Bahçeşehir Üniversitesi, Tıp Fakültesi (2019-2022)
7. Anabilim Dalı Başkanı, Biyofizik, Bahçeşehir Üniversitesi Tıp Fakültesi, (2014-2022)
8. Fakülte Yönetim Kurulu Üyesi, Bahçeşehir Üniversitesi, Tıp Fakültesi (2013-2022)
9. Disiplin Kurulu Üyesi, Bahçeşehir Üniversitesi, Tıp Fakültesi (2013-2022)

10. Bilimsel ve Mesleki Kuruluşlara Üyelikler

1. Kanada Biyofizik Derneği (2022 -)
2. Alman Biyofizik Derneği (2018-)
3. Türk Biyofizik Derneği (2016-)
4. Türk Kimya Derneği (2016 -)
5. Moleküler Grafik ve Modelleme Derneği- *Molecular Graphics and Modelling Society* (2013 -)
6. Amerika Biyofizik Derneği -*Biophysical Society* (2012 -)

7. Amerika Kimya Derneği- *American Chemical Society* (2012 -)
8. Kanada Kimya Derneği- *Canadian Society for Chemistry* (2012 -)

11. Ödüller

1. Bilime Katkı Ödülü, Bahçeşehir Üniversitesi (2023)
2. Topluma Katkı Ödülü, Bahçeşehir Üniversitesi (2021)
3. TÜSEB Aziz Sanar Teşvik Ödülü (2017)
4. TÜBİTAK Teşvik Ödülü (2016)
5. Bilim Akademisi BAGEP Ödülü (2014)
6. Bilime Katkı Ödülü, Bahçeşehir Üniversitesi (2016)

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	
2021-2022	Güz	TMED1000 (Biyofizik)	2	1	180
		MED2017 (Moleküler Modelleme ve Simülasyonlara Giriş)	2	1	12
	Bahar	TMED1000 (Biyofizik)	2	1	180
2022-2023	Güz	TMED1000 (Biyofizik)	2	1	180
		MED2043 (Antikanser İlaç Geliştirmede Makine Öğrenmesi Yöntemleri)	2	1	17
		PHAR1003 (Chemistry of Life)	3	3	26
	Bahar	TMED1000 (Biyofizik)	2	1	180
		PHAR1004 (Chemistry of Life)	3	3	30