Prof. Dr. Serdar DURDAĞI

Dean, School of Pharmacy

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I apply computational chemistry methods to biological systems. My interdisciplinary research projects focus on protein modeling and dynamics, ligand- and structure-based drug design, and the investigation of molecular mechanisms of protein-drug, protein-protein, and protein-DNA interactions, alongside optimization protocols for rational drug design. To support these aims, I utilize biophysical approaches and molecular modeling, and I also develop programming codes to address various biological problems. I have also established several startups in Boston and Istanbul that specialize in computer-aided drug design and development, such as Istanbul MedChem Inc. and ATPharma Inc. Additionally, I serve as the ambassador for Türkiye for the American Biophysical Society (BPS) during the 2024-2026 term.

Research Fields

- Ligand-based Drug Design
- Target-based Drug Design
- Machine-Learning-based QSAR models
- Pharmacophore Modeling
- ADME/Tox predictions
- Hit Identification
- Virtual screening of small molecule libraries
- MD simulations
- Molecular Docking
- Covalent Docking
- Lead Optimization
- Homology Modeling/Protein Engineering
- QM Calculations
- Steered MD simulations
- Programming

Work Experience

- Founding Dean and Professor
  Bahcesehir University (BAU), School of Pharmacy, Department of Pharmaceutical Chemistry
  April 2022 – Current

- Vice Dean, Head of Department of Basic Medical Sciences, and Professor
  Bahcesehir University (BAU), School of Medicine, Department of Biophysics
  September 2018 – April 2022

- Vice Dean, Head of Department of Biophysics, and Associate Professor
  Bahcesehir University (BAU), School of Medicine, Department of Biophysics
  December 2013 – September 2018

- Assistant Professor
  Bahcesehir University (BAU), School of Medicine, Department of Biophysics
  September 2013 – December 2013

- Senior Scientist
  Max Planck Inst. for Dynamics of Complex Technical Systems, Molecular Simulations and Design Group
  September 2012 – September 2013

- Canadian Institute of Health Research (CIHR) Fellow / Alberta Innovates Health Solutions (AIHS) Fellow; University of Calgary, Department of Biosciences
  January 2011 – March 2013

- Post Doctorate Fellow
  University of Calgary, Department of Biosciences
  April 2009 – March 2013

- EU Marie Curie Early Stage Researcher
  NHRF, Institute of Organic and Pharmaceutical Chemistry
  April 2006 – April 2009

- Researcher
  Fritz-Haber-Institute of Max-Planck Society, Theory Department
  February 2005 – April 2006

- Guest Researcher
  Innsbruck University, Theoretical and Inorganic Chemistry Department
  November 2004 – February 2005

Positions Offered

- Senior Researcher position (2013)
  Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

- Post Doctorate Fellow position (2011)
  Cambridge University, UNILEVER Centre for Molecular Sci. Informatics, Cambridge, U.K.

- Post Doctorate Fellow position (2009)
  Sydney University, School of Physics, Sydney, Australia

- Post Doctorate Fellow position (2009)
  University of Minnesota, Center for Drug Design, Minneapolis, U.S.A

Education

- **Ph.D.** (2006 - 2009)
  Pharmaceutical Chemistry / Computational Biophysics
  Free University of Berlin, Berlin (Germany)
  Ph.D. thesis awarded "**summa cum laude** -*with the highest honour*"
  Supervisors: Prof. Hartmut Oschkinat, Prof. Thomas Mavromoustakos

- **M.Sc.** (2002 - 2004)
  Computational Chemistry
  Bilkent University, Ankara (Türkiye)
  Supervisor: Prof. Ulrike Salzner

- **B.Sc.** (1997 - 2001)
  Chemistry
  Hacettepe University, Ankara (Türkiye)

- English Preparatory School (1996-1997)
  Hacettepe University, Ankara (Türkiye)

Personal Skills and Competence

Languages: Turkish (mother language), English (fluent), German (intermediate)

Leadership: Principal investigator and group leader since 2011, good experience in project and team management (currently responsible for a team of more than 50 people)

Technical Skills: Computer-aided drug design applications (molecular modeling, docking, MD simulations and post-MD analyses, machine learning based QSAR modeling, virtual screening, drug repurposing, protein engineering and modeling, programming/code development, Experience with RDKit, molecular simulations suites (Schrodinger, MOE, etc.), and docking programs (AutoDock Vina, rDock, gnina, etc.) Proficient in Python and the PyData stack (numpy, pandas, scipy, scikit-learn, etc.)

Computer Skills and Competences: Professional experience of Python, Tcl, awk, shell scripting

Application Programs and Software: Gaussian, GAMES, Gromacs, Turbomole, CASTEP, VASP, CHARMM, NAMD, AMBER, Desmond, Sybyl Molecular Modeling Package, Schrodinger Maestro Molecular Modeling package, MOE, FlexX, GOLD, AutoDock, ROSETTA, HADDOCK, etc.

Wet Lab Experience: High resolution and solid state NMR spectroscopy, 2D-NMR, Infrared (IR) spectroscopy, Differential Scanning Calorimetry (DSC), UV-Visible spectroscopy

Teaching Experience and Leadership Activities in Research Domain

- **Supervised PhD theses: (1)** Salmas, R.E. (2015); **(2)** Kayik, G. (2017); **(3)** Is, YS. (2019); **(4)** Aydin, G. (2020); **(5)** Aksoydan, B. (2021); **(6)** Al-Janabi, H. (2022); **(7)** Erol, I. (2023)

- **Supervised MSc theses: (1)** Kantarcioglu, I. (2017); **(2)** Tutumlu, G. (2019); **(3)** Sayin, V.O.; **(4)** Balkan, A. A. (2020); **(5)** Himmetoglu, A.(2020); **(6)** Oktay, L. (2020); **(7)** Yildiz, A. (2020); **(8)** M D Kamrul, H. (2021); **(9)** Tolu, I. (2022); **(10)** Motapanyane, N.B. (2022); **(11)** Ammuri, H. (2022); **(12)** Sambur, E. (2023); **(13)** Haddad, S. (2023); **(14)** Sayyah, E. (2023)

- **Undergraduate and graduate level courses offered (selected):** Physical Biochemistry (Univ. Of Calgary, 2011-2012); Molecules of Life (BAU, 2014-2017); Special Topics in Bioinformatics (BAU, 2014-2017); Biophysics (BAU, 2014-2023); Introduction to Molecular Modeling and Simulations (2015-2023); Machine Learning Application in AntiCancer Drug Design (2018-2023); Chemistry of Life (BAU, 2022-2024)

Memberships

- American Association for Cancer Research -AACR *(2019- current)*
- Biophysical Society -BPS *(2009 – current)*
- Canadian Society for Chemistry *(2009 – present)*
- Biophysical Society of Canada (2009- current)
- Biophysical Society of Germany (2020- current)
- American Chemical Society *(2012 – present)*
- Molecular Graphics and Modeling Society *(2013 – present)*

Editorial Board

- *Frontiers in Chemistry* (Associate Editor, 2022-present)
- *All Life* (Section Editor, 2019- present)
- *Turkish Journal of Biology* (2017 – present)
- *Current Enzyme Inhibition* (2015 - present)
- *Frontiers in Medicinal and Pharmaceutical Chemistry* (2014 –present)
- *BMC Pharmacology and Toxicology* (2014-present)
- *Turkish Journal of Chemistry* (2013 – present)
- *Biochemistry and Pharmacology* (2012 – present)
- *E Journal of Chemistry* (2012 – present)
- *Journal of Enzyme Inhibition and Medicinal Chemistry* (2011 – 2018)

Publications

1. Kahveci, K., Duzgun, M.B., Atis, A.E., Yilmaz, A., Shahraki, A., Coskun, B., **Durdagi, S.,** Iyison, N.B. Discovering allotastatin type-C receptor specific agonists. ***Nature Communications.*** 2024, 15, 3965. DOI:10.1038/s41467-024-48156-w.

2. Mavroedi, P., Zorba, L.P., Tzouras, N.V., Neofotistos, S.P., Georgiou, N., Sahin, K., **Durdagi, S**., Vougioukalakis, G.C., Mavromoustakos, T. Are terminal alkynes necessary for MAO-A/MAO-B inhibition? A new scaffold is revealed. ***Molecules*** 2024, 29, 2486.

3. Sayyah, E., Oktay, L., Tunc, H., **Durdagi, S.** Developing Dynamic Structure-based Pharmacophore and ML-Trained QSAR Models for the Discovery of Novel Resistance-Free RET Tyrosine Kinase Inhibitors. ***ChemMedChem*** 2024 (accepted)

4. Ikram, S., Sayyah, E., **Durdagi, S.** Identifying Potential SOS1 Inhibitors via Virtual Screening of Multiple Small Molecule Libraries against KRAS-SOS1 Interface. **ChemBioChem** 2024 (accepted)

5. Ghazy, S., Oktay, L., **Durdagi, S.** A novel algorithm for the virtual screening of extensive small molecule libraries against ERCC1/XPF protein-protein interaction for the identification of therapeutic resistance-bypassing small anticancer molecules. ***Turk. J. Biol.*** 2024 (accepted)

6. Kekecmuhammed, H., Tapera, M., Sahin, K., Ozturk Sever, B., Anber, A.M., Bora, R.E., Avsar, T., Kilic, T., Gunger, E., Saripinar, E., Coker-Gurkan, A., **Durdagi, S**. The suppressive effect of novel hydrazones-tethered imidazoles in HCT-116 and HT-29 colorectal cancer cells: Synthesis, biological activity, and molecular modeling studies. ***ChemistrySelect*** 2024 (accepted)

7. Cakmak, R., Basaran, E., Sahin, K., Senturk, M., **Durdagi, S**. Synthesis of Novel Hydrazide-Hydrazone Compounds and in vitro and in silico Investigation of their Biological Activities against AChE, BChE, and hCA I and II. ***ACS Omega***. 2024, 9, 18, 20030-20041.

8. Ozil, M., Balaydin, H.T., Dogan, B., Senturk, M., **Durdagi, S**. 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. Arch. Pharm. 2024, e2300266. DOI: 10.1002/ardp.202300266.

9. Sambur, E., Oktay, L., **Durdagi, S**. Covalent docking-driven virtual screening of extensive small-molecule libraries against Bruton tyrosine kinase for the identification of highly selective and potent novel therapeutic candicates. ***J. Mol. Graph. Model.*** 2024, 130, 108762. DOI: 10.1016/j.jmgm.2024.108762.

10. Sukkar B., Oktay, L., Sahaboglu A., Moayedi A., Zenouri S., Tamer Al-Maghout, Cantó, A., Miranda M., **Durdagi, S**., Hosseinzadeh Z. Inhibition of altered Orai1 channel in Müller cells rescues Photoreceptor in degenerated retina. ***Glia*** 2023 (accepted)

11. 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.

12. 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.

13. 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.

14. 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

15. 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.

16. 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.

17. 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.

18. 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.

19. 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.

20. 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.

21. 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.

22. **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.

23. 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.

24. 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.

25. 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.

26. **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.

27. 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.

28. 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.

29. 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.

30. **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

31. 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.

32. 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.

33. **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, DeMirci 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.

34. 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.

35. 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.

36. 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.

37. 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.

38. 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.

39. Kanan, T., Kanan, D., Jaffar, I., **Durdagi, S.** Transcription Factor NF-κB as Target for SARS-CoV-2 Drug Discovery Efforts Using Inflammation-based QSAR Screening Model (2021) ***Journal of Molecular Graphics and Modelling*** 108, pp107968.

40. 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.

41. 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.

42. 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

43. 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.

44. Shahraki, A., Işbilir, A., Dogan, B., Lohse, M.J., **Durdagi, S.,** Birgul-Iyison, N. Structural and Functional Characterization of Allatostatin Receptor Type-C of Thaumetopoea pityocampa, a Potential Target for Next-Generation Pest Control Agents (2021) ***Journal of Chemical Information and Modeling***, 61 (2), pp. 715-728.

45. 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.

46. 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

47. Akbayrak, I.Y., Caglayan, S.I., **Durdagi, S.,** Kurgan, L., Uversky, V.N., Ulver, B., Dervisoğlu, 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

48. 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/acsptsci.0c00210

49. 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.

50. Onder, FC., **Durdagi, S.,** Kahraman, N., Uslu, TN., Kandemir, H., Atici, EB., 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

51. Avsar, T., Yigit, BN., Turan, G., Altunsu, D., Calis, S., Kurt, B., Kilic, T., Ergun, MY., **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.

52. 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.jmgm.2020.107727

53. 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.jmgm.2020.107744

54. 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.jmgm.2020.107720

55. 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

56. 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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16. Mestanoglu, M.; Gokdemir, E.; Salmas, R.E.; **Durdagi, Serdar**. **3rd Anticancer Drug Development Congress.** Rehabilitating Drug-induced Long-QT Promoters-II: De Novo Design of hERGneutral Anti-Cancer Drugs with Retained Restrictive Effects on Cell Proliferation. ***Turkey,* 2015.**

17. **Durdagi, Serdar**; Ergun, G.; Gokdemir, E.; Salmas, R.E.; Ergun, M.Y.; Bulut, G. **GRC Computer Aided Drug Design Congress** Structure-based Designed New Generation Anti-hypertensive Oxazalone and Imidazolone Derivatives and Investigation of Their Potential Restrictive Effects On Cell Proliferation. ***U.S.A.*, 2015**

18. Rosenhouse-Dantsker, Avia; Noskov, Sergei; **Durdagi, Serdar**; Logothetis, Diomedes E.; Levitan, Irena. Identification of Novel Cholesterol Binding Regions in the Transmembrane Domain of Kir2.1. *Biophysical Journal*, 106(2), 747A- 747A, **2014**.

19. **Durdagi, Serdar;** Patterson, M.; Noskov, SY. **58th Annual Biophysical Society Meeting.** *Biophysical Journal* "Development and validation Studies of Universal Pharmacophore Models for hERG Channel Openers" ***U.S.A., 2014.***

20. **Durdagi, Serdar**. **10th Nano science and Nanotechnology Conference** "Multi-scale Modeling, Molecular Simulations and Nanoscale Analysis to Design Novel K-RAS-PDEδ Interaction Inhibitors as Anti-Cancer Drugs" ***Turkey,* 2014**.

21. Buturak, Birce; **Durdagi, Serdar**; Noskov, Sergei Y.; Ozal Ildeniz, A.T. **2nd International BAU Drug Design Congress** "In Silico Designing of Multi-Targeted Molecules" ***Turkey*, 2014**

22. **Durdagi, Serdar**. **2nd International BAU Drug Design Congress** "Rehabilitating Drug- induced Long-QT Promoters: In Silico Design of hERG Non-Blocker Compounds with Retained Pharmacological Activity Using Molecular Surgery Studies" ***Turkey,* 2014**

23. Salmas, R.E.; Unlu, A.; **Durdagi, Serdar**; Yurtsever, M.; Noskov, S.Y. **2nd International BAU Drug Design Congress** "Structural Variation of PARP-1 over Inhibitory Treatment, Holo State Definitional from Apo Form: Approaching MD and Docking Simulations" ***Turkey,* 2014**

24. Salmas, R.E.; **Durdagi, Serdar**; Stein, M.; Yurtsever, M. **2nd International BAU Drug Design Congress** "In Silico Study of Approved Antipsychotic Drugs as D2R Antagonists: Homology Modeling and Docking Approach" ***Turkey,* 2014**

25. Zervou, Maria; Cournia, Zoe; Potamitis, Constantinos; Patargias, George; **Durdagi, Serdar**; Grdadolnik, Simona G., Mavromoustakos, Thomas. **247th ACS National Meeting and Exposition** "Molecular Basis of Action of the AT1 Antagonist Losartan" ***U.S.A.,* 2014**

26. **Durdagi, Serdar**; Randal, Trevor; Duff, Henry J.; Noskov, Sergei Y. **57th Annual Biophysical Society Meeting** *Biophysical Journal* "Rehabilitation Studies For Withdrawn Drugs From The Market: Derivation Of Non-Herg1 Channel Blocker Cisapride Analogues Using Multi-Faceted Approaches, ***U.S.A.,* 2013**.

27. Noskov, S.Y.; **Durdagi, Serdar**; Perissinotti, L.; Duff, H.J. **Drug Discovery and Therapy World Congress** "Multi-Scale Approach To Modeling Drug Blockade and Activation of hERG Channel" ***U.S.A.,* 2013**.

28. **Durdagi, Serdar**; Yazdi, S.; Stein, M. **6th Theoretical Biophysics Symposium** "Analysis of Protein-Protein Interactions of the Site-specific Mono and tetra-Ubiquitin-associated IκBα/NF-κB Complexes" ***Sweden,* 2013**.

29. Yazdi, S.; **Durdagi, Serdar**; Stein, M. **6th Theoretical Biophysics Symposium** "The interplay between phosphorylation of IκBα and its recognition by β-TrCP through MD simulation and protein-protein docking" ***Sweden,* 2013**.

30. **Durdagi, Serdar**; Yazdi, S.; Stein, M. **27th Molecular Modeling Workshop** "Protein- Protein Docking Analysis and Refinement of the Ubiquitin- and Tetraubiquitin-associated IkBa/NF-kB Complexes", ***Germany,* 2013**.

31. **Durdagi, Serdar**. **1st International BAU Drug Design Symposium "**Rehabilitation Studies for Withdrawn Drugs from the Market Using Multi-Scale Modeling Approaches" ***Turkey,* 2013**.

32. **Durdagi, Serdar**; Deshpande S.; Duff H.; Noskov S. **95th Canadian Chemistry Conference and Exhibition** "Protein Engineering Studies for the Derivation of Atomistic Models of Open, Closed and Open-Inactivated States of hERG1 Channel using ROSETTA Protein Modeling Suite and Molecular Dynamics Simulations" ***Canada,* 2012**.

33. **Durdagi, Serdar**; Duff, H; Noskov, S, **4th International Congress on Cell Membranes and Oxidative Stress** kongresi dahilinde Cell Membranes And Free Radical Research dergisinde "Modeling and Validation Studies of Open, Closed and Open-inactivated States of hERG1 Channel: A Multi-faceted Approach" *19*, ***Turkey,* 2012**

34. **30. Durdagi, Serdar**. **3rd Kananaskis Symposium on Theoretical Models in Chemistry and Biology** "Recent Advances in Protein-Protein Docking algorithms" ***Canada,* 2012.**

35. Agelis, George; Resvani, Amalia; **Durdagi, Serdar**; Tumova, Tereza; Slaninov, J.; Giannopoulos, Phillip; Spyridaki, Katerina; Liapakis, George; Vlahakos, Demetrios; Mavromoustakos, Thomas; Matsoukas, John. **European Peptide Symposium** *Journal Of Peptide Science* "A Concise Synthesis, Docking Studies and Biological Evaluation of N- Substituted 5-Butylimidazole Analogues as Potent Angiotensin II Receptor Blockers" *18*, S116, **2012.**

36. **Durdagi, Serdar**; Deshpande, S; Duff, H; Noskov, SY. **56th Annual Biophysical Society Meeting** *Biophysical Journal* "Development of Atomistic Models of Open, Closed and Open- Inactivated States of hERG1 Channel using ROSETTA Protein Modeling Suite and Molecular Dynamics Simulations", *679*, ***U.S.A.,* 2012**.

37. **Durdagi, Serdar**; Noskov, Sergei Y. "Consistency of constructed hERG1 pore domain and pharmacophore models: A 3D-QSAR, molecular docking, and pharmacophore modeling study" *Biochemistry and Cell Biology-Biochimie et Biologie Cellulaire*, 89(2), 266-267, **2011**.

38. **Durdagi, Serdar**. **ROSETTA Protein Modeling Workshop** Vanderbilt University, Nashville, ***U.S.A.,* 2011**

39. Zoumpoulakis P., **Durdagi, Serdar**, Potamitis C., Kritsi E., Golic Grdadolnik S., Mavromoustakos T **12th Conference Medicinal Chemistry** "Comparative studies between Telmisartan and other AT1 antagonists at membrane and receptor active site" ***Greece*, 2011**

40. **Durdagi, Serdar**; Duff, Henry J.; Noskov, Sergei Yu. **Ion Channels, Gordon Research Conference** "Molecular Modeling and Validation Studies of the hERG1 Pore and Voltage Sensing Domains with ROSETTA-Membrane and Molecular Dynamics Simulations" ***U.S.A.,* 2010**

41. **Durdagi, Serdar**; Noskov, Sergei Yu. **53rd Annual Meeting of the Canadian Society for Biochemistry, Molecular and Cellular Biology: Membrane Proteins in Health and Disease** *Biochemistry and Cell*

Biology "Consistency of constructed hERG1 pore domain and pharmacophore models: A 3D QSAR, molecular docking and pharmacophore modeling study", 266, ***Canada,* 2010**.

42. Zoumpoulakis, P.; **Durdagi, Serdar**; Potamitis, C.; Kritsi, E.; Golic Grdadolnik S.; Mavromoustakos T. **14th Hellenic Symposium on Medicinal Chemistry** "Comparative conformational analysis and docking studies between Telmisartan and valsartan. Insights on the molecular basis of action of their pharmacophores associated with AT1 antagonism" ***Greece*, 2010**.

43. **Durdagi, Serdar**. **1st Kananaskis Computational Biology Symposium** "hERG Blockers and Activators" ***Canada,* 2010.**

44. **Durdagi, Serdar**; Zoumpoulakis, P. Reis, H.; Papadopoulos, M. G.; Koukoulitsa, C.; Papahatjis, D. P.; Mavromoustakos, T. **9th International Conference in Medicinal Chemistry-Drug Discovery and Design *Greece* 2008.**

45. Mavromoustakos T.; **Durdagi, Serdar**; Papahadjis, D.; Papadopoulos, M.G., **4th Hellenic Crystallographic Association Conference** "X-ray diffraction studies combined with molecular dynamics calculations to study the effects of cannabinoids in lipid bilayers and CB receptor active site" 23, ***Greece,* 2008**

46. **Durdagi, Serdar**; Zoumpoulakis, P.G.; Reis, H.; Papadopoulos, M.G.; Koukoulitsa, C.; Papahatjis, D.P.; Mavromoustakos, T. **13th Hellenic Symposium of Medicinal Chemistry** "Molecular Docking and Molecular Dynamics Simulations of the potent Δ8- THC analogue AMG3" ***Greece,* 2008.**

47. Politi, A.; **Durdagi, Serdar**; Papavasilopoulou, E.; Moutevelis-Minakakis, P.; Kokotos, G.; Mavromoustakos, T. **13th Hellenic Symposium of Medicinal Chemistry** "3D QSAR/CoMFA and CoMSIA Studies of Aliskirens" ***Greece,* 2008.**

48. Mavromoustakos, T., Petrou, C.; Kokkalou, E.; Roussis, V.; Christofi, V.; Efthimio, G.; Potamitis, C.; **Durdagi, Serdar**; Mavromoustakos, S. "**7th Joint Meeting of the Association-Francophone pour l'Enselgnement-et-la-Recherce-en- Pharmacognosie/American Society of Pharmacognosy/Society for Medical Plant Research/Pythochem Society of Europe"** "Ficus Sycomoros Sap: A Psoralene Source with Potential for the Treatment of Psoriasis" *Planta Medica*, 74, 9, 1006, ***Greece,* 2008**.

49. **Durdagi, Serdar**; Zoumpoulakis, P.; Papadopoulos, M.G.; Mavromoustakos, T. **6th Hellenic Forum on Bioactive Peptides** "Conformational Analysis and Computational Refinement of H1-NMR Spectra of AT1 Antagonists Losartan and Irbesartan Using MD Simulations and ONIOM method" ***Greece,* 2008**

50. Mavromoustakos, T.; **Durdagi, Serdar**. **6th Hellenic Forum on Bioactive Peptidesm**"Peptide Mimetics and their Interdigitation with Lipid Bilayers" ***Greece* ,2008**

51. **Durdagi, Serdar**. **Molecular Modeling workshop: Approaches to Computational Biophysics**, National Hellenic Research Foundation, ***Greece***

52. **Durdagi, Serdar**. **Structure-based Drug Discovery Workshop**, National Hellenic Research Foundation, ***Greece,* 2008**.

53. **Durdagi, Serdar**; Zoumpoulakis, P. Reis, H.; Papadopoulos, M. G.; Koukoulitsa, C.; Papahatjis, D. P.; Mavromoustakos, T. **9th International Conference in Medicinal Chemistry-Drug Discovery and Design** "Synergetic use of 3D QSAR, Molecular Docking and Molecular Dynamics Simulations at the Conformational Analysis of Drugs" ***Greece,* 2008.**

54. Mavromoustakos, T., Petrou, C.; Kokkalou, E.; Roussis, V.; Christofi, V.; Efthimio, G.; Potamitis, C.; **Durdagi, Serdar**; Mavromoustakos, S. "**7th Joint Meeting of the Association-Francophone pour l'Enselgnement-et-la-Recherce-en- Pharmacognosie/American Society of Pharmacognosy/Society for Medical Plant Research/Pythochem Society of Europe"** "Ficus Sycomoros

Sap: A Psoralene Source with Potential for the Treatment of Psoriasis" *Planta Medica*, 74, 9, 1006, ***Greece,*** **2008**.

55. **Durdagi, Serdar**; Koukoulitsa, C.; Zoumpoulakis, P.; Kapou, A.; Kourouli, T.; Andreou, T.; Nikas, S. P.; Nahmias, V. R.; Papahatjis, D. P.; Papadopoulos, M. G.; Mavromoustakos, T., **6th AFMC International Medicinal Chemistry Congress** Drugs Of The Future "Testing the 3D QSAR CoMFA/CoMSIA Results of Flexible Bioactive Compounds with Molecular Docking", 79, ***Turkey,*** **2007**

56. Mavromoustakos, Thomas; Zervou, Maria; Zoumpoulakis, Panagiotis G.; Potamitis, Costas; Katsiaris, Vassilis; Politi, Aggeliki; Mantzourani, Efthimia; **Durdagi, Serdar**, Koukoulitsa, Catherine. **6th AFMC International Medicinal Chemistry Congress** *Drugs Of The Future* "Putative Bioactive Conformers of Small Molecules: A Concerted Approach Using NMR Spectroscopy and Computational Chemistry", 33, ***Turkey,*** **2007**

57. **Durdagi**, **Serdar**; Koukoulitsa, C.; Zoumpoulakis, P; Papadopoulos M. G.; Papahatjis, D. P.; Mavromoustakos, T. **2nd Hellenic Symposium, Organic Synthesis-From Chemistry to Biology, Medicine and Material Science** "An Algorithm for the Conformational Analysis of Flexible Drug Molecules: A Critical Aspect for the 3D-QSAR Studies and Rational Drug Design" ***Greece,*** **2007.**

58. **Durdagi, Serdar**; Koukoulitsa, C.; Kapou, A.; Kourouli, T. Andreou, T.; Nikas, S.P.; Nahmias, V.R.; Papahatjis, D.P.; Papadopoulos, M.G.; Mavromoustakos, T. **8th International Conference in Medicinal Chemistry-Drug Discovery and Design** "The Applications of 3D-QSAR and Pharmacokinetic Studies for the Novel Cannabinoid Ligands Substituted at the C1' Position of the Alkyl Side Chain" ***Greece*** **2007**.

59. **Durdagi, Serdar**; Koukoulitsa, C.; Kourouli, T.; Andreou, T.; Nikas, S. P.; Nahmias, V. R.; Papahatjis, D. P.; Papadopoulos, M. G.; Mavromoustakos, T., "**EURO-QSAR2006, 16th European Symposium on Quantitative Structure-Activity Relationships & Molecular Modeling**" Euro-Qsar2006 "Theoretical Investigation of Pharmacokinetic Profile of Synthetic Cannabinoids" ***Italy,*** **2006.**

60. **Durdagi, Serdar**; Kaplan Can, H.; Guner, A. **2nd European Medical & Biological Engineering Conference, Advancement of Medicine and Health Care, EMBEC'02** "Adsorption-desorption studies of BSA on DEAE/Dextran", ***Austria*** **2002**.

Books

1. Mavromoustakos, Thomas; Tzakos, Andreas G.; **Durdagi, Serdar**. Supramolecules in Drug Discovery and Drug Delivery Methods and Protocols Preface. *Supramolecules in Drug Discovery and Drug Delivery: Methods and Protocols*, 2207, V-V, **2021**.

2. **Durdagi**, **S.** Recent Advances in Computational Drug Design Studies: The Application of *In Silico* Methodologies For Bioactive Cannabinoid and Fullerene Derivatives, VDM-Verlag, **2010**

Chapters in Books

1. Kiriakidi, Sofia; Kolocouris, Antonios; Liapakis, George; Ikram, Saima; **Durdagi, Serdar**; Mavromoustakos, Thomas. Effects of Cholesterol on GPCR Function: Insights from Computational and Experimental Studies. *Direct Mechanisms in Cholesterol Modulation of Protein Function*, 1135, 89-103, **2019**.

2. Erol, Ismail; Aksoydan, Busecan; Kantarcioglu, Isik; **Durdagi, Serdar**. Application of Multiscale Simulation Tools on GPCRs. An Example with Angiotensin II Type 1 Receptor. *Rational Drug Design Methods and Protocols*, 1824, 431-448, **2018**.

3. Tzoupis, Haralambos; Avramopoulos, Aggelos; Reis, Heribert; Leonis, Georgios; **Durdagi, Serdar**; Mavromoustakos, Thomas; Megariotis, Grigorios; Papadopoulos, Manthos G. Theoretical Studies of Interactions in Nanomaterials and Biological Systems. *Towards Efficient Designing of Safe Nanomaterials: Innovative Merge of Computational Approaches and Experimental Techniques*, 25, 148-185, **2013**.

4. **Durdagi, S**.; Roux, B.; Noskov, S.Y. *Encylcopedia Of Metalloproteins* "Potassium-Binding Site Types in Proteins" 1809-1815, **2013**

5. Deshpande, S.; **Durdagi, S**.; Noskov, S. *Encylcopedia Of Metalloproteins* "Potassium in Biological Systems" 1799-1804, **2013**
6. Mavromoustakos, T.; Moutevelis-Minakakis, P.; Kokotos, G.; Papavassilopoulou, E.; Potamitis, C.; Fotakis, C.; Chatzigeorgiou, F. Vyras, K.; Koukoulitsa, C.; Kalatzis, E.; **Durdagi, S**. *Essays On Contemporary Peptide Science* **2011**
7. Tzoupis, H.; Avramopoulos, A.; Reis, H.; Leonis, G.; **Durdagi**, **S**.; Mavromoustakos, T.; Megariotis, G.; Papadopoulos, M.G. Theoretical Studies Of Interactions In Nanomaterials And Biological Systems*. Towards Efficient Designing Of Safe Nanomaterials: Innovative Merge Of Computational Approaches And Experimental Techniques.* Jerzy Leszczynski ve Tomasz Puzyn (Ed.). The Royal Society of Chemistry, **2012**

Selected Awards

1. The Turkish Academy of Sciences (TÜBA) **Academy Award** in Health and Life Sciences (2023)
2. The Turkish Academy of Sciences (TÜBA) **Academy Medal** (2023)
3. Bahcesehir University (BAU) 25th Year Special Science Award (2023)
4. Contribution to Science Award, BAU (2023)
5. Social Benefit Award, BAU (2021)
6. Health Institutes of Turkey- TUSEB's **Aziz Sancar Incentive Award** (2017)
7. The Scientific and Technological Research Council of Turkey (**TUBITAK**) **Incentive Award** in Health Sciences (2016)
8. Contribution to Science Award, BAU (2016)
9. Science Academy Young Scientist Award -BAGEP (2014)
10. The Scientific and Technological Research Council of Turkey (TÜBİTAK) / EU 7th Frame Work, Co-Funded Brain Circulation Program Award (2013)

Selected Invited Talks

- Durdagi, S. "Developing Dynamic Structure-Based Pharmacophore and ML-Based QSAR Models for the Discovery of New Anti-Cancer Therapeutics through Long Molecular Dynamics Trajectories and the Utilization of these Models in Accelerated Ligand Screening" ***EMBO Lecture Course***, Istanbul, Türkiye, 2023.
- Durdagi, S. "New methods in in silico methods to accelerate the transition from preclinical to clinical stage" ***University of Athens*****,** Greece, 2022.
- Durdagi, S. "Rehabilitating Drug-induced Long-QT Promoters: In Silico Design of hERG Non-Blocker Compounds with Retained Pharmacological Activity Using Molecular Surgery Studies" ***Bogazici University***, Faculty of Science, Istanbul, 2014.
- Durdagi, S. "Protein Engineering Studies on Ion Channels", ***Harvard University****, Harvard Medical School*, Boston, U.S.A, 2012.
- Durdagi, S. "Protein-Protein Docking Algorithms" ***Max-Planck Institute***, Magdeburg, Germany, 2012.
- Durdagi, S. "Ligand and Structure-based Drug Design Studies" ***Zurih University***, Faculty of Medicine, Zurich, Switzerland, 2011.
- Durdagi, S. "Recent Advances on Drug Design Studies" ***The European Molecular Biology Laboratory-EMBL***, Heidelberg, Germany, 2011.
- Durdagi, S. "Development of Pharmacophore Models for hERG1 Blockers and Openers" ***Novo Nordisk Foundation Center for Protein Research***, Copenhagen University, Denmark, 2011.

External Reviewer of Scientific Journals (selected)

- *Nature Communications*
- *Nature Chemical Biology*
- *Journal of Chemical Information and Modeling*
- *Journal of Medicinal Chemistry*
- *iScience*
- *Bioorganic and Medicinal Chemistry*
- *Bioorganic and Medicinal Chemistry Letters*
- *PLOS One*
- *European Journal of Medicinal Chemistry*
- *Biophysical Journal*
- *Journal of Computer Aided Molecular Design*
- *BBA Biomembranes*
- *Journal of Molecular Graphics and Modelling*
- *Journal of Enzyme Inhibition and Medicinal Chemistry*
- *Journal of Biomolecular Structure and Dynamics*
- *Frontiers in Chemistry*
- *RSC Medicinal Chemistry*

External Reviewer of Science Foundations (selected)

- Innovates Medicine Initiative (IMI), European Union (EU)
- Swiss National Science Foundation
- National Science Centre Poland
- Vienna Science and Technology Fund (Austria)
- Austrian Science Fund
- The Latvian Council of Science
- The Scientific and Technological Research Institution of Türkiye (TÜBİTAK)
- National Health Institutes of Türkiye (TÜSEB)
- Science Academy (Türkiye)
- European Union EuroStars Expert (EU)
- EUREKA Expert (EU)