Prof. Dr. Serdar DURDAĞI

Biophysics / Computational Biophysics

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Research Group of Dr. Durdagi applies computational chemistry methods to biological systems. Inter-disciplinary research of group focuses on protein modeling and dynamics, ligand- and structure-based drug design, investigation of molecular mechanisms of protein/drug, protein/protein, protein/DNA interactions and optimizations protocols for rational drug design. For this aim, together with applications of biophyscial approaches and molecular modeling applications research Lab of Dr. Durdagi also developes programing codes for several biological problems.

Work Experience

- September 2018 -Current
  Professor
  Bahcesehir University (BAU), School of Medicine
  Department of Biophysics, Istanbul, Turkey

- December/2013 –September 2018
- **Assoc. Professor**
  Bahcesehir University (BAU), School of Medicine
  Department of Biophysics, Istanbul, Turkey

- October/2012 – December/2013
- **Assist. Professor**
  Bahcesehir University (BAU), School of Medicine
  Department of Biophysics, Istanbul, Turkey

- September/2012 - August 2013
- **Senior Scientist**
  Max Planck Institute for Dynamics of Complex Technical Systems
  Molecular Simulations and Design Group, Magdeburg, Germany

- January/2011 – March/2013
- **Canadian Institute of Health Research (CIHR) Fellow**
- **Alberta Innovates Health Solutions (AIHS) Fellow**
  University of Calgary
  Department of BioSciences, Institute for Biocomplexity and Informatics. Calgary, Alberta, Canada

- April/2009 – March/2013
- **Post-Doctorate Associate**
  University of Calgary
  Department of BioSciences, Institute for Biocomplexity and Informatics. Calgary, Alberta, Canada

- April/2006 – April/2009
- **European Union Marie-Curie Early Stage Researcher** (under EU 6th Frame-Work project)
  The National Hellenic Research Foundation
  Institute of Organic and Pharmaceutical Chemistry, Computational Chemistry Lab. Athens, Greece

- February/2005 – April/2006
- **Researcher**
  Fritz-Haber-Institute of Max-Planck Society
  Theory Department. Berlin, Germany

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

- September/2004 – October/2005
- **Teaching and Research Assistant**
  Bilkent University
  Department of Chemistry, Computational Chemistry Lab. Ankara, Turkey

Positions Offered

- **University of Cambridge,** Dept. of Chemistry, UNILEVER Centre for Molecular Sci. Informatics, Cambridge, U.K., Post-Doctorate Fellowship position
- **Maastricht University, Cardiovascular Research Institute** Maastricht, Netherlands, Post-Doctorate Fellowship position
- **University of Sydney**, School of Physics Sydney, Australia, Post-Doctorate Fellowship position
- **University of Minnesota**, Twin Cities, Center for Drug Design Minneapolis, U.S.A., Post-Doctorate Fellowship position
- **Max Planck Institute for Dynamics of Complex Technical Systems** Molecular Simulations and Design Group, Magdeburg, Germany

Education/Training

Dates	01/04/2006 - 09/05/2009
Title of Qualification Awarded	**Ph.D.**
Principal Subjects	Biophysics / Computational Biophysics
University	**Free University of Berlin,** Berlin (Germany) Ph.D. thesis awarded "**summa cum laude -*with the highest honour***" (Supervisors: Prof. Hartmut Oschkinat, Prof. Thomas Mavromoustakos)
Dates	01/09/2002 – 01/10/2004
Title of Qualification Awarded	**M.Sc.**
Principal Subjects	Computational Chemistry –*Education Language was in English*
University	Bilkent University, Ankara (Turkey) (Supervisor: Prof. Ulrike Salzner)
Dates	15/09/1997 – 01/08/2001
Title of Qualification Awarded	**B.Sc.**
Principal Subjects	Chemistry –*Education Language was in English*
University	Hacettepe University, Ankara (Turkey)
Dates	15/09/1996 – 01/07/1997
Principal Subjects	English Preparatory School
University	Hacettepe University, Ankara (Turkey)

Personal Skills and Competence

Mother Language	**Turkish**
Other Languages	**English (fluent), German (pre-intermediate), Greek (basic)**
Organisational Skills and Competences	• Leadership (PI since 2011) • Good experience in project and team management (Currently responsible for a team of 10 people)
Technical Skills and Competences	Computer-aided drug design (structure-based and ligand-based); Pharmacophore modeling; Homology modeling; 3D-QSAR; 4D-QSAR; Molecular docking (Protein/Ligand; Protein-Protein); Molecular dynamics simulations; *De novo* drug design; Structure elucidation; Conformational analysis; ADMET applications; MM and QM applications to biological systems; De novo receptor and Loop modeling; Programming-Code development (Python, C, Fortran, etc.) • Professional experience of following programming languages:

Computer Skills and Competences

Python, C, JAVA, Tcl, Fortran, awk, shell scripting

- Professional experience of Microsoft Office tools (Word, Excel and PowerPoint, etc.)
- Professional experience of Operating Systems Linux, UNIX, Windows, Mac.

Application Programs and Software

Gaussian 03/09; GAMES; GROMACS; TURBOMOLE; CASTEP; VASP; CHARMM; NAMD; VolSurf (ADMET property prediction); SYBYL Molecular modeling package (3D QSAR/CoMFA, CoMSIA; MULTISEARCH; LEAPFROG (De Novo Design); MOLCAD; BIOPOLYMER; CLUSTERING modules, etc.); FlexX Docking; AutoDock; GOLD Docking; ClusPro; HADDOCK; ROSETTA Protein modeling; SCHRODINGER Molecular modeling Package (Glide, IFD; PHASE, Macromodel; Prime, Jaguar, Maestro, etc.); O2; Origin; Molekel; VMD; Pymol, VegaZZ; ChemPlus; Xmgrace; HyperChem, etc.

Wet Lab Experiences

- High resolution and solid-state NMR spectroscopy
- Infrared (IR) spectroscopy
- Differential Scanning Calorimetry (DSC)
- UV-Visible Spectroscopy
- High Pressure Liquid Chromatography-Gel Permeation Chromatography (HPLC-GPC)

Research Interests

- Ion Channels (K channels (i.e., hERG; KcsA; Kv1.2, etc.)
- GPCRs (CB1 and CB2 receptors, Angiotensin-II (AT1) receptor; β_2-adrenergic receptor, etc.)
- HIV-1 protease and its inhibitors
- C60 (Fullerene) and Its Derivatives for Different Biological Applications
- Carbonic Anhydrase (CA) enzymes and their inhibitors
- Nanoporous structures (Carbon nanotubes, graphene, etc.)
- KRAS/PDEδ Inhibitors as Anti Cancer Agents
- poly ADP ribose polymerase (PARP) Inhibitors
- Mono and tetra-Ubiquitin-associated IκBα/NF-κB Complexes
- Force Field Development
- Structural and dynamical properties of ions (Bi^{3+}, Li^{+}, Ca^{2+} etc.) in different solvents

Memberships

- Biophysical Society -BPS *(2012 – present)*
- Canadian Society for Chemistry *(2012 – present)*
- American Chemical Society *(2012 – present)*
- Molecular Graphics and Modeling Society *(2013 – present)*

<u>Administrative:</u>

- Member of Clinical Research and Ethics Committee, BAU School of Medicine *(2013 – present)*
- Scientific Communucation Committee Member, BAU School of Medicine *(2013 – present)*
- Education Commission Member, BAU School of Medicine *(2013 – present)*
- Publication Ethics Board Member, BAU School of Medicine *(2013 – present)*
- Vice Dean, BAU School of Medicine *(2014 – present)*

Editorial Board

- *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 - present)
- *Current Enzyme Inhibition* (2015 - present)
- *Turkish Journal of Biology* (2017 – present)

Publications

1. Ntountaniotis, D.; Andreadelis, I. ; Kellici, T.; Karageorgos, V.; Leonis, G.; Christodoulou, E.; Kiriakidi, S.; Becker-Baldus, J.; Stylos, E.; Chatziathanasiadou, M. ; Chatzigiannis, C. ; Damalas, D.; **Durdagi, S**.; Javornik, U.; Valsami, G.; Glaubitz, C; Aksoydan, B.; Thomaidis, N.; Kolocouris, A.; Plavec, J.; Tzakos, A.; 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*** (accepted)

2. Kiriakidi, S.; Kolocouris, A.; Liapakis, G.; Ikram, S.; **Durdagi, S.***, Mavromoustakos, T. Effects of cholesterol on GPCR function. **(2019) ADVANCES IN EXPERIMENTAL MEDICINE AND BIOLOGY** (accepted)

3. Tarek Kanan, Duaa Kanan, Ismail Erol, Samira Yazdi, Matthias Stein, **Serdar Durdagi*.** Targeting the NF-ϰB/IϰBα Complex via Fragment-Based E-Pharmacophore Virtual Screening and Binary QSAR Models. **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING** 2018 (accepted)

4. Ramin Ekhteiari Salmas, Philip Seeman, Matthias Stein, **Serdar Durdagi***. Structural Investigation of the Dopamine-2 Receptor (D2R) Agonist Bromocriptine Binding to Dimeric D2HighR and D2LowR States. **JOURNAL OF CHEMICAL INFORMATION AND MODELING** 2018 (accepted)

5. Yusuf Serhat Is, **Serdar Durdagi***, Busecan Aksoydan, Mine Yurtsever. Proposing Novel MAO-B Hit Inhibitors Using Multidimensional Molecular Modeling Approaches and Application of Binary QSAR Models for Prediction of their Therapeutic Activity and Toxic Effects. **ACS CHEMICAL NEUROSCIENCE** 2018 (accepted)

6. **Serdar Durdagi***, Ismail Erol, Ramin Ekhteiari Salmas, Busecan Aksoydan, Isik Kantarcioglu. Oligomerization and Cooperativity in GPCRs from the Perspective of the Angiotensin AT1 and Dopamine D2 Receptors. **NEUROSCIENCE LETTERS** 2018 (accepted)

7. Ismail Erol, Busecan Aksoydan, Isik Kantarcioglu, **Serdar Durdagi***. Application of Multiscale Simulation Tools on GPCRs. An Example with Angiotensin II Type I Receptor. **METHODS IN MOLECULAR BIOLOGY** 2018

8. **Serdar Durdagi*,** Muhammad Tahir ul Qamar, Ramin Ekhteiari Salmas, Quratulain Tariq, Farooq Anwar, Usman Ali Ashfaq. Investigating the Molecular Mechanism of Staphylococcal DNA Gyrase Inhibitors: A Combined Ligand-based and Structure-based Resources Pipeline. **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING** 2018

9. Mehreen Zaka, Bilal Haider Abbasi, **Serdar Durdagi***. Proposing Novel TNFα Direct Inhibitor Scaffolds Using Fragment-Docking based e-Pharmacophore Modeling and Binary QSAR-based Virtual Screening Protocols Pipeline. **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING** 2018

10. Mehreen Zaka, Bilal Haider Abbasi, **Serdar Durdagi***. 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. **JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS** 2018

11. Adriano Mollica,Gokhan Zengin, **Serdar Durdagi**, Ramin Ekhteiari Salmas, Giorgia Macedonio, Azzurra Stefanucci, Marilisa Pia Dimmito, Ettore Novellino. Combinatorial Peptide Library Screening for Discovery of Diverse α-glucosidase Inhibitors Using Molecular Dynamics Simulations and Binary QSAR Models. **JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS** 2018

12. Ilkay Erdogan Orhan, Dariusz Jedrejek, F. Sezer Senol, Ramin Ekhteiari Salmas, **Serdar Durdagi,** Iwona Kowalska, Lukasz Pecio, Wieslaw Oleszek: Molecular Modeling and In vitro Approaches Towards Cholinesterase Inhibitory Effect of Some Natural Xanthohumol, Naringenin, and Acyl Phloroglucinol Derivatives. **PHYTOMEDICINE** 2018

13. **Serdar Durdagi*,** Busecan Aksoydan, Ismail Erol, Isik Kantarcioglu, Yavuz Ergun, Gulay Bulut, Melih Acar, Timucin Avsar, George Liapakis, Vlasios Karageorgos, Ramin E. Salmas, Barış Sergi, Sara Alkhatib, Gizem Turan, Berfu Nur Yigit, Kutay Cantasir, Bahar Kurt, and Turker Kilic **(2018)** Integration of Multi-scale Molecular Modeling Approaches with Experiments for the in silico Guided Design and Discovery of Novel hERG-Neutral Antihypertensive Oxazalone and Imidazolone Derivatives and Analysis of Their Potential Restrictive Effects on Cell Proliferation. **EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY** 145, 273-290.

14. Maria Joao Rodriques, Sylwester Slusarczyk, Lukasz Pecio, Adam Matkowski, Ramin E. Salmas, **Serdar Durdagi**, Caterina G. Pereira, Joao C. Varela, Luisa A. Barreira, Lusia Custodio **(2018)** In vitro and in silico approaches to appraise Polygonum maritimum L. as a soruce of innovative products with anti-aging potential. **INDUSTRIAL CROPS AND PRODUCTS** 111, 391-399.

15. Kayik, G.; Senyurt Tuzun, N.; **Durdagi, S.* (2017)** Structural Investigation of Vesnarinone at the Pore Domains of Open and Open-Inactivated States of hERG1 K^+ Channel. **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING.** DOI: 10.1016/j.jmgm.2017.08.017

16. Aksoydan, B.; Kantarcioglu, I.; Erol, I.; Salmas, R.E.; **Durdagi, S.* (2017)** Structure-based Design of hERG-Neutral Antihypertensive Oxazolone and Imidazolone Derivatives. **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING.** DOI: 10.1016/j.jmgm.2017.08.004

17. Akincioglu, A.; Kocaman, E.; Akincioglu, H.; Salmas, R.E.; **Durdagi, S.;** Gulcin, I.; Supuran, C.T; Goksu, S. **(2017)** The Synthesis of Novel Sulfamides Derived from beta-Benzylphenethylamines as Acetylcholinesterase, Butyrylcholinesterase and Carbonic Anhydrase Enzymes Inhibitors. **BIOORGANIC CHEMISTRY.** DOI: 10.1016/j.bioorg.2017.08.012

18. Mirza S.B,; Hua Leed R.G.; Hann Chud, J.G.; Salmas, R.E.; Mavromoustakos, T.; **Durdagi, S.* (2017)** Discovery of Selective Dengue Virus Inhibitors Using Combination of Molecular Fingerprint-Based Virtual Screening Protocols, Structure-based Pharmacophore Model Development, Molecular Dynamics Simulations and *in Vitro* Studies. **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING.** DOI: 10.1016/j.jmgm.2017.08.006

19. Salmas, R.E.; Is, Y.S.; **Durdagi, S**.; Stein, M.; Yurtsever, M. **(2017)** A QM Protein-Ligand Investigation of Anti-psychotic Drugs with the Dopamine D2 Receptor (D2R) **JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS** DOI: 10.1080/07391102.2017.1365772

20. Zengin Kurt, B.; Sonmez, F.; **Durdagi, S*.;** Aksoydan, B.; Salmas, R.E.; Angeli, A.; Kucukislamoglu, M.; Supuran, C.T. (2017) Synthesis, Biological Activity and Multiscale Molecular Modeling Studies for Coumaryl-carboxamide Derivatives as Selective Carbonic Anhydrase IX Inhibitors***. Journal of Enzyme Inhibition and Medicinal Chemistry.*** DOI: 10.1080/14756366.2017.1354857

21. Salmas, R.E.; Gulhan, M.F.; **Durdagi, S**.; Sahna, E.; Abdullah, H.I.; Selamoglu, Z. **(2017)** Effects of Propolis, Caffeic Acid Phenethyl Ester and Pollen on Renal Injury in Hypertensive Rat: An Experimental and Theoretical Approach. **CELL BIOCHEMISTRY & FUNCTION.** DOI: 10.1002/cbf.3277

22. Erol, I.; Aksoydan, B.; Kantarcioglu, I.; Salmas, R.E.; **Durdagi, S.* (2017)** Identification of Novel Serotonin Reuptake Inhibitors Targeting Central and Allosteric Binding Sites: A Virtual Screening and Molecular Dynamics Simulations Study. **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING.** DOI: 10.1016/j.jmgm.2017.02.001

23. Erdemli, M.E.; Salmas, R.E.; **Durdagi, S**.; Akgul, H.; Demirkol, M.; Aksungur, Z.; Selamoglu, Z. **(2017)** Biochemical Changes Induced by Grapeseed Extract and Low Level Laser Therapy Administration During Intraoral Wound Healing in Rat Liver: An Experimental and in Silico Study. **JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS** DOI: 10.1080/07391102.2017.1305297.

24. **Durdagi, S***.; Erol, I.; Salmas, R.E.; Patterson, M.; Noskov, S.Y. **(2017)** First Universal Pharmacophore Model for hERG1 K+ Channel Activators. **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING.** DOI: 10.1016/j.jmgm.2017.03.020

25. Salmas, R.E.; Seeman, P.; Aksoydan, B.; Erol, I.; Kantarcioglu, I.; Stein, M.; Yurtsever, M.; **Durdagi, S.* (2017)** Analysis of the Glutamate Agonist LY404,039 Binding to Non-Static Dopamine Receptor D2 Dimer Structures and Consensus Docking. **ACS CHEMICAL NEUROSCIENCE** DOI: 10.1021/acschemneuro.7b00070

26. Bukiye, A.N.; **Durdagi, S**.; Noskov, S.Y.; Rosenhouse-Dantsker **(2017)** Cholesterol Up-regulates Neuronal G Protein-Gated Inwardly Rectifying Potassium (GIRK) Channel Activity in the Hippocampus. **JOURNAL OF BIOLOGICAL CHEMISTRY**. DOI: 10.1074/jbc.M116.753350

27. Salmas, R.E.; **Durdagi, S**.; Gulhan, M.F.; Duruyurek, M.; Abdullah, H.; Selamoglu, Z. **(2017)** The Effects of Pollen, Propolis, and Caffeic Acid Phenethyl Ester on Tyrosine Hydroxylase Activity and Total RNA Levels in Hypertensive Rats Caused by Nitric Oxide Synthase Inhibition: Experimental, Docking and Molecular Dynamic Studies**. JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS** DOI: 10.1080/07391102.2017.1288660.

28. Salmas, R.E.; Seeman, P.; Aksoydan, B.; Stein, M.; Yurtsever, M.; **Durdagi, S*. (2017)** Biological Insights of the Dopaminergic Stabilizer ACR16 at the Binding Pocket of Dopamine D2 Receptor. ***ACS CHEMICAL NEUROSCIENCE DOI:*** 10.1021/acschemneuro.6b00396

29. Kocak, R.; Akin, E.T.; Kalin, P.; Talaza, O.; Saracoglu, N.; Dastan, A.; Gulcin, I.; **Durdagi, S**. **(2016)** Synthesis of some novel norbornene-fused pyridazines as potent inhibitors of carbonic anhydrase and acetylcholinesterase. **JOURNAL OF HETEROCYCLIC CHEMISTRY** DOI: 10.102/jhet.2558

30. Shityakov, S.; Salmas, RE., **Durdagi, S**.; Salvador, E.; Papai, K.; Yanez-Gascon, M.; Sanchez-Perez, H.; Puskas, I.; Roewer, N.; Forster, C.; Broscheit, J-A. **(2016)** "Characterization, In Vivo Evaluation and Molecular Modeling of Different Propofol-Cyclodextrin Complexes to Assess Their Drug Delivery Potential at The Blood-Brain Barrier Level" **JOURNAL OF CHEMICAL INFORMATION AND MODELING (ACS)**, 56, 1914-1922.

31. Wang, Y.; Guo, J.; Perissinotti, L.; Lees-Miller, J.; Teng, G.; **Durdagi, S**.; Duff, HJ.; Noskov, S.Y. **(2016)** "Role of the pH in state-dependent blockade of hERG currents. **SCIENTIFIC REPORTS (NATURE)** doi:10.1038/srep32536

32. Shityakov, S.; Salmas, RE., **Durdagi, S**.; Roewer, N.; Forster, C.; Broscheit, J. **(2016)** "Solubility profiles, hydration and desolvation of curcumin complexed with γ-cyclodextrin and hydroxypropyl-γ-cyclodextrin" ***JOURNAL OF MOLECULAR STRUCTURES*** doi: 10.1016/j.molstruc.2016.12.028

Publications (Cont.)

33. Kayik, G.; Senyurt Tuzun, N.; **Durdagi, S**. **(2016)** "Investigation of PDE5/PDE6 and PDE5/PDE11 Selective Potent Tadalafil-like PDE5 Inhibitors Using Combination of Molecular Modeling Approaches, Molecular Fingerprint-Based Virtual Screening Protocols and Structure-based Pharmacophore Development" **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY,** *DOI:* 10.1080/14756366.2016.125075

34. Salmas, RE.; Stein, M.; Yurtsever, M.; Seeman, P.; Erol, I.; Mestanoglu, M.; **Durdagi, S**. **(2016)** "The Signaling Pathway of Dopamine D2 Receptor (D2R) Activation Using Normal Mode Analysis (NMA) and the Construction of Universal Pharmacophore Models for D2R Inhibitors" **JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS**; DOI: 10.1080/07391102.2016.1206487

35. Salmas, RE.; Unlu, A.; Bektas, M.; Yurtsever, M.; Mestanoglu, M.; **Durdagi, S. (2016)** "Virtual Screening of Small Molecules Databases for Discovery of Novel PARP-1 Inhibitors: Combination of in silico and in vitro Studies. **JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS***, DOI:* 10.1080/07391102.2016.1199328

36. Mirza, SB; Salmas, RE.; Fatmi, MQ; **Durdagi, S. (2016)** "Discovery of Klotho Peptide Antagonists Against Wnt3 and Wnt3a Target Proteins Using Combination of Protein Engineering, Protein-Protein Docking, Peptide Docking and Molecular Dynamics Simulations. **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY**; DOI: 10.1080/14756366.2016.1235569

37. Kayik, G.; Senyurt Tuzun, N.; **Durdagi, S**. **(2016) "**In Silico Design of Novel hERG-neutral Sildenafil-like PDE5 Inhibitors" **JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS** doi: 10.1080/07391102.2016.1231634

38. Kellici, TF.; Ntountaniotis, D.; Kritsi, E.; Zervou, M.; Zoumpoulakis, P.; Potamitis, C.; **Durdagi, S**.; Salmas, R.E.; Ergun, G.; Gokdemir, E.; Halabalaki M.; Gerothanassis, I.P.; Liapakis, G.; Tzakos, A.; Mavromoustakos, T. **(2016**) "Leveraging NMR and X-ray Data of the Free Ligands to Build Better Drugs Targeting GPCRs: The Case of AT1R" **CURRENT MEDICINAL CHEMISTRY** 23(1):36-59.

39. Ozgeris, B.; Goksu, S.; Kose, LP; Gulcin, I.; Salmas, RE.; **Durdagi, S.;** Tumer, F.; Supuran, CT. **(2016)** "Acetylcholinesterase and Carbonic Anhydrase Inhibitory Properties of Novel Urea and Sulfamide Derivatives Incorporating Dopaminergic 2-Aminotetralin Scaffolds. **BIOORGANIC AND MEDICINAL CHEMISTRY** 24, 2318-2329

40. Mirza, SB; Salmas, RE.; Fatmi, MQ; **Durdagi, S. (2016)** "Virtual Screening of Eighteen Million Compounds against Dengue Virus: Combined Molecular Docking and Molecular Dynamics Simulations Study" **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING** 66, 99-107.

41. Sahin, A.; Senturk, M.; Salmas, RE.; **Durdagi, S**.; Ayan, A.; Karagolge, A.; Mestanoglu, M. **(2016)** "Investigation of inhibition of human glucose 6-phosphate dehydrogenase by some 99mTc chelators by in silico and in vitro methods" **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY.** DOI: 10.1080/14756366.2016.1178735

42. Salmas, R.E.; Yurtsever, M.; **Durdagi, S. (2016)** "Atomistic Molecular Dynamic Simulations of Typical and Atypical Anti-psychotic Drugs at the Dopamine D2 Receptor (D2R) Elucidates Their Inhibition Mechanism" **JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS.** DOI: 10.1080/07391102.2016.1159986

43. **Durdagi, S**.; Salmas, R.E.; Stein, M.; Yurtsever, M.; Seeman, P. **(2016)** "Binding Interactions of Dopamine and Apomorphine in D2High and D2Low States of human Dopamine D2

Receptor (D2R) using Computational and Experimental Techniques" **ACS CHEMICAL NEUROSCIENCE** DOI: 10.1021/acschemneuro.5b00271

44. Fidan, I.; Senturk, M.; Arslan, M.; **Durdagi, S**.; Ekinci, D.; Cosgun, S. **(2015)** "Carbonic anhydrase inhibitors: design, synthesis, kinetic, docking and molecular dynamics analysis of novel glycine and phenylalanine sulphonamide derivatives" **BIOORGANIC & MEDICINAL CHEMISTRY** *23*, 7353-7358.

45. Isik, S.; Vullo, D.; **Durdagi, S**.; Ekinci, D.; Senturk, M.; Cetin, A.; Supuran, C.T. **(2015)** "Carbonic anhydrase inhibitory and activatory properties of some pyridine and phenol hydrazine carbothioamide derivatives" **BIOORGANIC & MEDICINAL CHEMISTRY LETTERS** *25*, 5636-5641.

46. Salmas, RE.; Mestanoglu, M.; Yurtsever, M.; Noskov, S.Y.; **Durdagi, S.* (2015)** "Mutated Form (G52E) of Inactive Diphtheria Toxin CRM197: Molecular Simulations Clearly Display Effect of the Mutation to NAD Binding" **JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS;** DOI: 10.1080/07391102.2015.1119060

47. Salmas, R.E.; Mestanoglu, M.; Yurtsever, M.; Noskov, S.Y.; **Durdagi, S* (2015)** "Molecular Simulations of Solved Co-crystallized X-ray Structures Identifies Action Mechanisms of PDEδ Inhibitors" **BIOPHYSICAL JOURNAL** 109, 1163-1168.

48. Salmas, R.E.; Yurtsever, M.; **Durdagi, S.* (2015)** "Investigation of Inhibition Mechanism of Chemokine Receptor CCR5 by Micro-second Molecular Dynamics Simulations" **SCIENTIFIC REPORTS (NATURE PG)**; DOI: 10.1038/srep13180

49. Salmas, R.E.; Yurtsever, M.; **Durdagi, S*. (2015)** "Protein Engineering Studies for C-C Chemokine Receptor Type 2 (CCR2)" **CURRENT ENZYME INHIBITION** DOI: 10.2174/1573408011666150807190410

50. Strom, T.A.; **Durdagi, S**.; Ersoz, S.S.; Salmas, R.E.; Supuran, C.T.; Barron, A.R. **(2015)** "Fullerene-based Inhibitors of HIV-1 Protease" **JOURNAL OF PEPTIDE SCIENCE** DOI 10.1002/psc.2828

51. **Durdagi, S.;** Korkmaz, N.; Isik, S.; Vullo, D.; Astley, D.; Salmas, R.E.; Ekinci, D.; Senturk, M.; Supuran, C.T. **(2015)** Kinetic and docking studies of cytosolic/tumor-associated carbonic anhydrase isozymes I, II, and IX with some hydroxylic compounds **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY** DOI: 10.3109/14756366.2015.1114930

52. Yazdi, S.; **Durdagi, S**.; Naumann, M.; Stein, M. **(2015)** "Structural modelling of the N-terminal signal-receiving domain of IkBa" **FRONTIERS IN MOLECULAR BIOSCIENCES**; DOI: 10.3389/fmolb.2015.00032

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Patents

- Systems and Methods of Selecting Compounds With Reduced Risk Of Cardiotoxicity Using hERG Models (**WIPO Patent, Patent No: WO 2016201566 A1)**

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25. **Durdagi, S**.; Duff, H.J.; Noskov, S.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**

26. **Durdagi, S**.; Noskov, S.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**.

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

28. Zoumpoulakis, P.; **Durdagi, S**.; 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**.

29. Mavromoustakos T.; **Durdagi, S**.; 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**

30. **Durdagi, S**.; 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.**

31. Politi, A.; **Durdagi, S.;** 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.**

32. **Durdagi, S**.; 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.**

33. Mavromoustakos, T., Petrou, C.; Kokkalou, E.; Roussis, V.; Christofi, V.; Efthimio, G.; Potamitis, C.; **Durdagi, S.;** 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**.

34. **Durdagi, S**.; 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**

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

36. **Durdagi, S. Molecular Modeling workshop: Approaches to Computational Biophysics**, National Hellenic Research Foundation, ***Greece* 2008**

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

38. **Durdagi, S**.; 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**

39. Mavromoustakos, T.; Zervou, M.; Zoumpoulakis, P.G.; Potamitis, C.; Katsiaris, V.; Politi, A.; Mantzourani, E.; **Durdagi, S**., Koukoulitsa, C. **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**

40. **Durdagi**, **S;** 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.**

41. **Durdagi, S**.; 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.**

42. **Durdagi, S.;** 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**.

43. **Durdagi, S. 3. Ilac Kimyasi Kongresi** "Uzun Moleküler Dinamik Simülasyonlar ile hERG İyon Kanal Açıcılarının Kanal Bağlanma Bölgelerinde Dinamik ve Yapısal Etkilerinin İncelenmesi ve Yeni hERG Kanal Açıcılarının Keşfi" *Antalya,* **2015.**

44. **Durdagi, S.;** Patterson, M.; Noskov, S.Y. **2. Ilac Kimyasi Kongresi** "hERG Iyon Kanali Acicilarinin Tasarimi icin Genel Farmakofor Modellerin Gelistirilmesi ve Validasyon Calismalari" *Antalya,* **2014.**

45. **Durdagi, S.;** Guo, J.; Changalov, M.; Perissinotti, LL.; Hargreaves, J.M.; Back, T.M.; Noskov, S.Y.; Duff, H.J. **25. Ulusal Biyofizik Kongresi** "hERG1 Potasyum Kanal Agonisti NS1643 ve Turevlerinin Yapı-Fonksiyon Analizleri ve Moleküler Mühendislik Çalışmaları: Sentez, Elektrofizyoloji, Ligand ve Yapı-Bazlı İlaç Tasarım Çalışmaları Kombinasyonu" Trabzon, **2013**.

46. Ekhteiari Salmas, R.; **Durdagi, S.;** Stein, M.; Yurtsever , M. **25. Ulusal Biyofizik Kongresi** "Dopamin (D2) Reseptorünün Aktif ve İnaktif Konformasyonlarının Protein Modelleme Teknikleri ile Geliştirilmesi ve Validasyonu: Şizofreni Tedavisinde Kullanılan Standart İlaçların Moleküler Mekanizmalarının Aydınlatılması" Trabzon, **2013**.

47. **Durdagi, S**; Duff, H.J.; Noskov, S. **25. Ulusal Kimya Kongresi** "Recent Advances on Computer Aided Drug Design Studies" Erzurum, **2011**

48. Şentürk, M.; Ekinci, D.; **Durdagi, S**. **25. Ulusal Kimya Kongresi** "Bazı Organik Bileşikler ve Amino Asitlerin İnsan Asetilkolinesteraz ve Butirilkolinesteraz Enzimleri Üzerindeki İnhibisyon Kinetiği ve Mekanizması" Erzurum, **2011.**

49. Ekinci, D.; Şentürk, M.; **Durdagi S**. **International Conference on Enzyme Science and Technology** "Biological activity and molecular modeling studies of some natural compounds as α and β-glycosidase inhibitors", Kuşadası, **2011**

50. **Durdagi, S**.; Kaplan Can, H.; Guner, A. **15. Ulusal Kimya Kongresi** "BSA'in çapraz bağlı Dietilaminoetil mikro küreleri üzerine adsorpsiyonu" İstanbul, **2001**.

Books

Durdagi, S.; "**Recent Advances in Computational Drug Design Studies**: The Application of In Silico Methodologies for Bioactive Cannabinoid and Fullerene Derivatives" **2010**, published by VDM-Verlag, Germany, ISBN: 978-3-639-22256-2

Chapters in Books

- **Durdagi, S**.; Roux, B.; Noskov, S.Y. ENCYLCOPEDIA OF METALLOPROTEINS "Potassium-Binding Site Types in Proteins" 1809-1815, 2013
- Deshpande, S.; **Durdagi, S**.; Noskov, S. ENCYLCOPEDIA OF METALLOPROTEINS "Potassium in Biological Systems" 1799-1804, 2013
- 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**
- 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**
- Mavromoustakos, T.; Golic Grdadolnik, S.; Zervou, M.; Zoumpoulakis, P.; Potamitis, C.; Politi, A.; Mantzourani, E.; Platts, J.A.; Koukoulitsa, C.; Minakakis, P.; Kokotos, G.; Tselios, T.; Matsoukas, J.; **Durdagi**, **S.;** Papadopoulos, M. G.; Papahatjis, D.P.; Spyranti, Z.S.; Dalkas, G.A.; Spyroulias, G.A. MEDICINAL CHEMISTRY RESEARCH PROGRESS "Putative Bioactive Conformers of Small Molecules: A Concerted Approach Using NMR Spectroscopy and Computational Chemistry", 175-205, Colombo, G. P.; Ricci, S. (Ed.) **2009**
- Salzner, U.; Karalti, O.; **Durdagi, S**, Clark, T. HIGHLIGHTS IN COMPUTATIONAL CHEMISTRY II "Does the Donor–Acceptor Concept Work for Designing Synthetic Metals? Theoretical Investigation of Copolymers between Quinoid Acceptors and Aromatic Donors", 687-702, **2006**.

Teaching Experience and Leadership Activities in Research Domain

a. Supervised 10 PhD students and 15 undergraduate students on short-term research projects
b. Attended "Instructional Skills Workshop" at the Teaching and Learning Centre of the University of Calgary (24 hours, March 2010).

- I am teaching Biophysics Lectures at the School of Medicine, Bahcesehir University
- I was responsible for teaching three chapters at the "*Biomolecular Simulations*" course-a graduate students level course- at the Department of Biological Sciences/University of Calgary. In this course, I was also responsible to teach two Labs in Computer-Aided Drug Design and Molecular Docking. In this Lab, I taught applications of one of the most commonly used molecular docking program AutoDock to 26 students (2012).
- I taught (as invited Lecturer) two chapters in the "*Molecular Biophysics*" course-a graduate s level course- at the Department of Biological Sciences/University of Calgary (2011).
- I gave several departmental seminars at the *Institute for Biocomplexity and Informatics* and I assisted several undergraduate and graduate students in their short-term projects. (2009 - 2012)
- I organized an international "Drug Design" conferences at the Bahcesehir University, Faculty of Medicine (2013) and I organized "2nd, 3rd, 4th and 5th International Drug Design Congress" (2014-2017) and "In Silico Techniques-I: 3D Protein Engineering" Workshops (2014)
- Invited for giving a talk and to be a Panel Chair at the 58th Biophysical Society Meetings, San Francisco, U.S.A. (2014)

- Invited and attended for "2nd Congress for Turkish Scientists Living Abroad" meeting organized by TUBITAK (2013) (Only 80 renown Turkish scientists from abroad are invited)

Awards and Scholarships

1. **Health Institutes of Turkey- TUSEB's Aziz Sancar Incentive Award (2017)**
2. **The Scientific and Technological Research Council of Turkey-TUBITAK's Incentive Award in Healthy Sciences (2016)**
3. **Contribution to Science Award (2016)**
4. **Science Academy's Young Scientist Award -BAGEP (2014) Science Academy "Young Scientists Award" for year of 2014.** (The priority of the Science Academy is to encourage young scientists to conduct sound scientific research and to award selected outstanding work. An award program has been initiated with a view to identify the best young academicians, to award and to support them in their new research efforts.) (2014)
5. **The Scientific and Technological Research Council of Turkey (TUBITAK) / EU 7th Frame Work, Co-Funded Brain Circulation Program Award** (2013)
6. **Max-Planck Institute Research Fellowship** (2012-2013)
7. **Canadian Institutes of Health Research (CIHR) Fellowship** (01/2011-03/2013)
8. **Alberta Innovates Health Solutions (AIHS) Fellowship** (01/2011-03/2013)
9. **Top-10 most cited paper for period of 2011-2012** (S. Durdagi et al, Bioorg. Med. Chem. *19*, 1381-1389, 2011)
10. **Top-25 downloaded paper for period of January-March 2011** (S. Durdagi et al, J. Mol. Graph. Model. *29*, 425-435, 2010)
11. **The top-10 most downloaded paper for the year of 2011** (S. Durdagi et al, J. Chem. Inf. Model. 51, 463-474, 2011)
12. **The most downloaded paper for period of January-March 2011** (S. Durdagi et al, J. Chem. Inf. Model. 51, 463-474, 2011)
13. **University of Calgary Post-Doctorate Fellowship**, (awarded by the Department of Biological Sci. of University of Calgary; 05/2009-present)
14. **6th Frame work of European Union, Marie-Curie Fellowship** (a full 3-years research grant, 04/2006-04/2009)
15. **The paper published at the J. Chem. Inf. Model** (49, 1139, 2009) **highlighted at the Nature Nanotechnology** journal (4, 401, 2009)
16. **Top-25 most downloaded article at the Bioorg Med Chem** (18, 2822, 2010)
17. **Top-25 most downloaded article at the Bioorg Med Chem Lett** (17, 6754, 2010)
18. **Full scholarship awarded by Max-Planck Institute**, Germany (02/2005-04/2007)
19. **The paper published at J. Mol. Model. (12, 687, 2006) has been selected as outstanding paper.**
20. **Full scholarship awarded by Austrian Science Foundation (FWF)** (11/2004-02/2005)
21. **Full scholarship, teaching and research assistantship awarded by Science and Engineering Inst. of Bilkent University** (09/2002-10/2004)
22. **Scientific meeting support program**, **The Scientific and Technological Research Council of Turkey (TUBITAK)** (12/2002-01/2003)
23. **The Union of Chambers Commerce, Industry, Trade and Commodity exchanges of Turkey (TOBB) higher education scholarship** (09/1997-09/1999)
24. **The Prime Ministry (Turkey) scholarship for higher education** (09/1996-08/2001)

External Reviewer of Scientific Journals (Selected)

- *Journal of Medicinal Chemistry*
- *Bioorganic and Medicinal Chemistry*
- *Bioorganic and Medicinal Chemistry Letters*
- *PLOS One*
- *Journal of Chemical Information and Modeling*
- *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*
- *Archiv der Pharmazie*
- *Chemosphere*

Selected Invited Talks

- **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.
- **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, Dermark, 2011.

Most Significant Research Contributions

Atomistic receptor models of hERG1 pore and voltage-sensing domains

The human ether-a-go-go related gene 1 (hERG1) K+ channel essential for the normal repolarization phase of the cardiac action potential. Single hERG1 channels are either closed, open or inactivated conformations. Since there is no crystal structure of hERG channels, creation and validation of reliable 3D models of ion channels has been a key target in molecular cardiology and pharmacology for the last decade. The atomistic receptor models help to understand their molecular mechanisms and thereby may assist to provide fresh insights into our understanding of functional roles of ion channels as well as have been valuable in defining functionally important domains of these proteins. We have developed *-first time literature-* the atomistic receptor models of pore and voltage sensing domains of the hERG1 potassium ion channel representing the open-state conformation (Proteins 2010) and derived model then called at the literature as "**Durdagi/Subbotina Model**". Although so far many models were built for the hERG channel, they all were limited to the pore domain. In our study, a full trans membrane model of the channel is developed. We tested a template-driven de novo design with ROSETTA-membrane modeling using side-chain placements optimized by subsequent molecular dynamics (MD) simulations. Although backbone templates for the homology modeled parts of the pore and voltage sensors were based on the available structures of KvAP, KcsA, Kv1.2 and Kv1.2-Kv2.1 chimera channels, the missing parts are modeled de-novo. In our recent studies, we also derived closed and open-inactivated states of hERG1 using ROSETTA protein modeling suite. (Durdagi et al., J. Chem Inf. Model 2012, Durdagi et al., JPET 2012)

Pharmacophore model development for studies of drug blockade and activation in the hERG1 Channel

Molecular modeling techniques can assist in screening drug candidates for their blocking and activation abilities to the hERG1 ion channel. Since the main idea of quantitative structure-activity relationships (QSAR) methods is to utilize a general pharmacophore model that can combine information of key functional groups of the ligand, an evaluation of the 3D-QSAR for hERG blockers and openers may assist to easy interpretation with quantitative analysis. For this aim, we created pharmacophore models for hERG blockers and for hERG openers. (Durdagi et al, J. Chem. Inf. Model. 2011)

Computer-aided drug design studies on anti-HIV

The inhibition of HIV type I aspartic protease (HIV-1 PR) by fullerene analogues has been proved and their complexations of HIV-1 PR has been supported by molecular modeling studies. However, the binding affinity values of fullerene inhibitors were not significant (Ki ~10^{-6} M). Thus, further structural investigation is required in order to propose new HIV-1 PR/fullerene complexes with optimal binding affinities. In part of my PhD studies, I have worked with fullerene derivatives at HIV-1 PR using several molecular modeling techniques such as 3D-QSAR, molecular docking, MD simulations and de novo drug design to predict high-affinity [60]fullerene derivative for HIV-1 PR. One of our proposed fullerene derivative as predicted anti-HIV drug has been proved by biological measurements and results showed that this fullerene derivative possess three times better potency than the currently existing fullerene-based anti-HIV ligand published in the literature. These studies have been published in the *J. Comput. Aided Mol. Des.* (25, 959, 2011); *J. Chem. Inf. Model.* (49, 1139, 2009) and published paper at JCIM is also highlighted at research highlights section of *Nature Nanotechnology* (4, 401, 2009) journal.

Combined 3D QSAR and molecular docking studies to reveal novel cannabinoid ligands with optimum binding activity

The knowledge of the receptor structure is not a pre-requisite for 3D-QSAR analysis, however, the availability of its crystal structure or 3D receptor model facilitates the structure alignment, and can provide statistically more reliable models. In my PhD studies, we constructed atomistic receptor models of the cannabinoid receptors, which assisted to improve the alignment of ligands used in QSAR models, and thereby improve the stability of constructed pharmacophore models. Results were used to reveal novel cannabinoid ligands with optimum binding activities. (J. Med. Chem. (50, 2875, 2007); Molecular Diversity (14, 257, 2010); *Bioorg. Med. Chem.* (16, 7377, 2008); and *Bioorg. Med. Chem. Lett.* (17, 6754, 2007).