Assoc. Prof. Dr. Serdar DURDAĞI

Biophysics / Computational Biophysics

Department of Biophysics, School of Medicine, Bahcesehir University (BAU)

E-mail: serdar.durdagi@med.bau.edu.tr Phone: +90 (216) 579 8217

www.durdagilab.com

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 tools such as homology modeling, 3D-QSAR, molecular docking, molecular dynamics (MD) simulations combined with post-processing analyses, cheminformatics, Monte-Carlo simulations, loop modeling, de novo drug design, ADME/Tox; research Lab of Dr. Durdagi also developes programing codes for several biological problems.

Work Experience

Dates	December/2013 – Current
Position Held	**Assoc. Professor**
Employer	**Bahcesehir University (BAU), School of Medicine**
	Department of Biophysics, Istanbul, Turkey
Dates	October/2012 – December/2013
Position Held	**Assist. Professor**
Employer	**Bahcesehir University (BAU), School of Medicine**
	Department of Biophysics, Istanbul, Turkey
Dates	September/2012 - August 2013
Position Held	**Senior Scientist**
Employer	**Max Planck Institute for Dynamics of Complex Technical Systems**
	Molecular Simulations and Design Group, Magdeburg, Germany
Dates	January/2011 – March/2013
Position Held	**Canadian Institute of Health Research (CIHR) Fellow**
Employer	**Alberta Innovates Health Solutions (AIHS) Fellow**
	University of Calgary
	Department of BioSciences, Institute for Biocomplexity and Informatics. Calgary, Alberta, Canada
Dates	April/2009 – March/2013
Position Held	**Post-Doctorate Associate**
Employer	**University of Calgary**
	Department of BioSciences, Institute for Biocomplexity and Informatics. Calgary, Alberta, Canada
Dates	April/2006 – April/2009
Position Held	**European Union Marie-Curie Early Stage Researcher** (under EU 6th Frame-Work project)
Employer	**The National Hellenic Research Foundation**
	Institute of Organic and Pharmaceutical Chemistry, Computational Chemistry Lab. Athens, Greece
Dates	February/2005 – April/2006
Position Held	**Researcher**
Employer	**Fritz-Haber-Institute of Max-Planck Society**
	Theory Department. Berlin, Germany
Dates	November/2004 – February/2005
Position Held	**Guest Researcher**
Employer	**Innsbruck University**
	Theoretical and Inorganic Chemistry Department, Innsbruck, Austria
Dates	September/2004 – October/2005
Position Held	**Teaching and Research Assistant**
Employer	**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.)

Computer Skills and Competences

- Professional experience of following programming languages:
  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)*

Administrative:

- 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. **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.

2. 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.

3. 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

4. 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

5. 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

6. 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

7. 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

8. 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

9. 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

10. 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

11. 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.

Publications (Cont.)

12. **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

13. 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

14. 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

15. 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.

16. 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

17. 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

18. 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.

19. 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

20. 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

21. 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

22. 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

23. 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.

Publications (Cont.)

24. 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
25. 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
26. 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.
27. 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
28. 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.
29. 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
30. 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
31. **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
32. 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.
33. 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.
34. 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
35. 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.
36. 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

Publications (Cont.)

37. 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
38. 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
39. **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
40. 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
41. Akincioglu, A.; Akincioglu, H.; Gulcin, I.; Supuran, C.T.; **Durdagi, S**.; Goksu, S. **(2015)** "Discovery of Potent Carbonic Anhydrase and Acetylcholine Esterase Inhibitors: Novel Sulfamoylcarbamates and Sulfamides Derived from Acetophenones" **BIOORGANIC & MEDICINAL CHEMISTRY**; DOI:10.1016/j.bmc.2015.04.019
42. Salmas, R.E.; Senturk, M.; Yurtsever, M.; **Durdagi, S.* (2015)** "Discovering Novel Carbonic Anhydrase Type IX (CA IX) Inhibitors from Seven Million Compounds Using Virtual Screening and In Vitro Analysis" **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY**; DOI:10.3109/14756366.2015.1036049
43. Guo, J.; Cheng, YM; Lees-Miller, JP.; Perissinotti, L.L.; Claydon, T.W.; Hull, C.M.; Thouta, S.; Roach, D.E.; **Durdagi, S**.; Noskov, S.Y.; Duff, H.J. **(2015)** "NS1643 Interacts around L529 of hERG to Alter Voltage Sensor Movement on the Path to Activation" **BIOPHYSICAL JOURNAL**; 108(6):1400-13. DOI:10.1016/j.bpj.2014.12.055
44. Salmas, R.E.; Mestanoglu, M.; **Durdagi, S**.; Senturk. M.; Kaya, A.A.; Celenk, E.K **(2015)** "Kinetic and in silico studies of hydroxy-based inhibitors of carbonic anhydrase isoforms I and II" **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY**; DOI:10.3109/14756366.2014.1003216
45. Salmas, R.E.; Yurtsever, M.; Stein, M.; **Durdagi, S.* (2015)** Modeling and protein engineering studies of active and inactive states of human dopamine D2 receptor (D2R) and investigation of drug/receptor interactions. **MOLECULAR DIVERSITY**; DOI:10.1007/s11030-015-9569-3
46. Salmas, R.E.; Unlu, A.; Yurtsever, M.; Noskov, S.Y.; **Durdagi, S.* (2015)** "In-Silico investigation of PARP-1 catalytic domains in holo and apo states for the design of high affinity PARP-1 inhibitors. **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY** DOI: 10.3109/14756366.2015.1005011
47. Iqbal, J.; Al-Rashida, M.; **Durdagi, S**.; Alterio, V; Di Fiore, A. **(2015)** "Recent Developments of Carbonic Anhydrase Inhibitors as Potential Drugs. **BIOMED RESEARCH INTERNATIONAL**; 2015:174178. DOI:10.1155/2015/174178
48. Kufareva, I.; Katritch, V.; Participants of GPCR Dock 2013, Stevens, RC.; Abagyan, R. **(2014)** "Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges" **STRUCTURE**, 22, 1120-1139 (doi: 10.1016/j.str.2014.06.012)
49. Guo, J.; **Durdagi, S**.; Changalov, M.; Perissinotti, L.; Hargreaves, JM.; Back TG.; Noskov, S.Y.; Duff, H.J. **(2014)** "Structure Driven Design of Novel Human Ether-a-go-go-related Gene Channel (hERG1) Activators" **PLOS ONE** 9(9), e105553 (doi: 10.1371/journal.pone.0105553)
50. **Durdagi, S**.; Randall, T.; Duff, HJ.; Chamberlin, A.; Noskov, S.Y. **(2014)** "Rehabilitating drug-induced long-QT promoters: In-silico design of hERG-neutral cisapride analogues with retained pharmacological activity" **BMC PHARMACOLOGY AND TOXICOLOGY** 15, 14 (doi: 10.1186/2050-6511-1514

Publications (Cont.)

51. Leonis, G.; Avramopoulos, A.; Salmas, R.E.; **Durdagi, S.;** Yurtsever, M.; Papadopoulos, MG. **(2014)** "Elucidation of Conformational States, Dynamics, and Mechanism of Binding in Human kappa-Opioid Receptor Complexes" **JOURNAL OF CHEMICAL INFORMATION AND MODELING**, 54, 2294-2308.
52. Goksu, S.; Naderi, A.; Akbaba, Y.; Kalin, P.; Akincioglu, A.; Gulcin, I.; **Durdagi, S**.; Salmas, R.E. **(2014)** "Carbonic Anhydrase Inhibitory Properties of Novel Benzylsulfamides Using Molecular Modeling and Experimental Studies" **BIOORGANIC CHEMISTRY**, 56, 75-82.
53. Buturak, B.; **Durdagi, S**.; Noskov, S.Y.; Ildeniz Ozal, T. **(2014)** "Designing of Multi-Targeted Molecules Using Combination of Molecular Screening and In Silico Drug Cardiotoxicity Prediction Approaches" **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING** 50, 16-34
54. Rosenhouse-Dantsker, A.; Noskov, S.; **Durdagi, S.;** Logothetis, D.E.; Levitan, I. **(2013)** "Identification of Novel Cholesterol-Binding Regions in Kir2 Channels" **JOURNAL OF BIOLOGICAL CHEMISTRY** 43, 31154-31164doi:10.1074/jbc.M113.496117
55. **Durdagi, S**.; Scozzafava, G.L Vullo, D.; Sahin, H.; Kolayli, S.; Supuran, C.T. **(2013)** "Inhibition of Mammalian Carbonic Anhydrases I-XIV Grayanotoxin III: Solution and In Silico Studies" **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY** 29, 469-475 (doi:10.3109/14756366.2013.804072)
56. Zervou, M.; Cournia, Z.; Potamitis, C.; Patargas, G.; **Durdagi, S.;** Grdadolnic, S.G.; Mavromoustakos, T. **(2013)** "Insights into the Molecular Basis of Action of the AT1 Antagonist Losartan Using a Combined NMR Spectroscopy and Computational Approach" **BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES** 1838, 1031-1046
57. Kritsi, E.; Potamitis, C.; **Durdagi, S**.; Zoumpoulakis, P.; Grdadolnik, S.; Mavromoustakos, T. **(2013)** "Molecular Insights into the AT1 Antagonism based on Biophysical and In Silico Studies of Telmisartan" **MEDICINAL CHEMISTRY RESEARCH** 22, 4842-4857.
58. Ekinci, D.; Fidan, I.; **Durdagi, S.;** Kaban, S.; Supuran, C.T. **(2013)** "Kinetic and In Silico Analysis of Thiazolidin-Based Inhibitors of α-Carbonic Anhydrase Isoenzymes" **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY** *28*, 370-374.
59. Talaz, O., Cavdar, H., **Durdagi, S.,** Azak, H. & Ekinci, D. **(2013)** "Synthesis of 1,4-bis(indolin-1-ylmethyl)benzene Derivatives and their Structure-Activity Relationships for the Interaction of Human Carbonic Anhydrase Isoforms I and II" **BIOORGANIC & MEDICINAL CHEMISTRY** *21*, 1477-1482.
60. Mavromoustakos, T., Agelis, G.; **Durdagi, S. (2013)** "AT1 Antagonists: A Patent Review (2008-2012)" **EXPERT OPINION ON THERAPEUTIC Patents** 23, 1483-1494.
61. Balaydin, H. T., **Durdagi, S.,** Ekinci, D., Senturk, M., Goksu, S.; Menzek, A. **(2012)** "Inhibition of Human Carbonic Anhydrase Isozymes I, II and VI with a Series of Bisphenol, Methoxy and Bromophenol Compounds" **JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY** 27, 467-475.
62. **Durdagi, S**.; Guo, J.; Lees-Miller, J.; Duff, H.J.; Noskov, S.Yu. **(2012)** "Structure-Guided Topographic Mapping and Mutagenesis to Elucidate Binding sites for the hERG1 Potassium Channel (KCNH2) Activator-NS1643" **Journal of Pharmacology and Experimental Therapeutics**, *342*, 441-452.
63. **Durdagi, S**.; Papadopoulos, M.G.; Mavromoustakos, T., **(2012)** "An Effort to Discover the Preferred Conformation of the Potent AMG-3 Cannabinoid Analog When Reaching the Active Sites of the Cannabinoid Receptors", **EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY** *47*, 44-51 DOI: 10.1016/j.ejmech.2011.10.015

Publications (Cont.)

64. Agelis, G.; Resvani, A.; **Durdagi, S**.; Spyridaki, K.; Tumova, T.; Slaninova, J.; Giannopoulos, P.; Vlahakos, D.; Liapakis, G.; Mavromoustakos, T.; Matsoukas, J. **(2012)** "The Discovery of New Potent Non-peptide Angiotensin II AT1 Receptor Blockers: A Concise Synthesis, Molecular Docking Studies and Biological Evaluation of N-Substituted 5-Butylimidazole Derivatives" **EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY** 55, 358-374

65. **Durdagi, S**.; Vullo, D.; Pan, P.; Kahkonen, N.; Maatta, J.A.; Hytonen, V.; Parkkila, S.; Supuran, C.T. **(2012)** "Protein-protein Interactions: Inhibition of Mammalian Carbonic Anhydrases I-XV with the Murine Inhibitor of Carbonic Anhydrase and Other Members of the Transferrin Family" **JOURNAL OF MEDICINAL CHEMISTRY** *55*, 5529-5535

66. **Durdagi, S**.; Deshpande, S.; Duff, H. J.; Noskov, S. Y. **(2012)** "Modeling of Open, Closed, and Open-Inactivated States of the hERG1 Channel: Structural Mechanisms of the State-Dependent Drug Binding" **JOURNAL OF CHEMICAL INFORMATION AND MODELING** *10*, 2760-2774

67. Tzoupis, H; Leonis, G.; **Durdagi, S** ; Mouchlis, V.; Mavromoustakos, T; Papadopoulos, MG, **(2011)** "Binding of Novel Fullerene Inhibitors to HIV-1 Protease: Insight Through Molecular Dynamics and Molecular Mechanics Poisson-Boltzmann Surface Area Calculations" **JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN** *25*, 959-976, DOI: 10.1007/s10822-011-9475-4

68. Cakmak, R ; **Durdagi, S**; Ekinci, D; Senturk, M; Topal, G. **(2011)** "Design, Synthesis and Biological Evaluation of Novel Nitroaromatic Compounds as Potent Glutathione Reductase Inhibitors", **BIOORGANIC & MEDICINAL CHEMISTRY LETTERS** *21*, 5398-5402. DOI: 10.1016/j.bmcl.2011.07.002

69. Ekinci, D.; Çavdar, H.; **Durdagi, S.;** Talaz, D.; Şentürk, M.; Supuran, C.T., **(2011)** "Structure–Activity Relationships for the Interaction of 5,10-dihydroindeno[1,2-b]indole Derivatives with Human and Bovine Carbonic Anhydrase Isoforms I, II, III, IV and VI", **EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY** *49*, 68-73. DOI: 10.1016/j.ejmech.2011.12.022

70. Mavromoustakos, T.; Chatzigeorgiou, P.; Koukoulitsa, C.; **Durdagi, S**. **(2011)** "Partial Interdigitation of Lipid Bilayers", **INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY** *111*, 1172-1183, DOI: 10.1002/qua.22610

71. Koukoulitsa, C; **Durdagi, S**; Siapi, E; Villalonga-Barber, C; Alexi, X; Steele, BR; Micha-Screttas, M; Alexis, MN; Tsantili-Kakoulidou, A; Mavromoustakos, T. **(2011)** "Comparison of Thermal Effects of Stilbenoid Analogs in Lipid Bilayers Using Differential Scanning Calorimetry and Molecular Dynamics: Correlation of Thermal Effects and Topographical Position with Antioxidant Activity", **EUROPEAN BIOPHYSICS JOURNAL WITH BIOPHYSICS LETTERS** *40*, 865-875. DOI: 10.1007/s00249-011-0705-4

72. **Durdagi, S**; Senturk, M; Ekinci, D; Balaydin, HT; Goksu, S; Kufrevioglu, O; Innocenti, A; Scozzafava, A; Supuran, C.T. **(2011)** "Kinetic and Docking Studies of Phenol-Based Inhibitors of Carbonic Anhydrase Isoforms I, II, IX And XII Evidence a New Binding Mode within the Enzyme Active Site", **Bioorganic & Medicinal Chemistry** *19*, 1381-1389. DOI: 10.1016/j.bmc.2011.01.016

73. **Durdagi, S**; Duff, HJ; Noskov, S.Y. **(2011)** "Combined Receptor and Ligand-Based Approach to the Universal Pharmacophore Model Development for Studies of Drug Blockade to the hERG1 Pore Domain", **JOURNAL OF CHEMICAL INFORMATION AND MODELING** *51*, 463-474, DOI: 10.1021/ci100409y

74. **Durdagi, S.;** Noskov, S.Y. **(2011)** "Mechanism of K+ /Na+ Selectivity in Potassium Channels from the Perspective of the Nonselective Bacterial Channel NaK" **CHANNELS** *5*, 198-201. DOI: 10.4161/chan.5.3.15873

Publications (Cont.)

75. Subbotina, J; Yarov-Yarovoy, V; Lees-Miller, J; **Durdagi, S**; Guo, JQ; Duff, HJ; Noskov, SY, **(2011)** "Structural Refinement of the hERG1 Pore and Voltage-Sensing Domains with ROSETTA-Membrane and Molecular Dynamics Simulations", **PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS** *78*, 2922-2934. DOI: 10.1002/prot.22815

76. Politi, A; **Durdagi, S**; Moutevelis-Minakakis, P; Kokotos, G; Mavromoustakos, T, **(2010)** "Development of Accurate Binding Affinity Predictions of Novel Renin Inhibitors Through Molecular Docking Studies", **JOURNAL OF MOLECULAR GRAPHICS AND MODELLING** *29*, 425-435

77. Mavromoustakos, T; **Durdagi, S**; Koukoulitsa, C.; Simcic, M; Papadopoulos, MG; Hodoscek, M; Grdadolnik, S.G. **(2011)** "Strategies in the Rational Drug Design", **CURRENT MEDICINAL CHEMISTRY** *18*, 2517-2530. DOI: 10.2174/092986711795933731

78. **Durdagi, S**; Zhao, C; Cuervo, JE; Noskov, S.Y. **(2011)** "Atomistic Models for Free Energy Evaluation of Drug Binding to Membrane Proteins" **CURRENT MEDICINAL CHEMISTRY** *18*, 2601-2611

79. **Durdagi, S**; Subbotina, J; Lees-Miller, J; Guo, J; Duff, HJ; Noskov, SY, **(2010)** "Insights into the Molecular Mechanism of hERG1 Channel Activation and Blockade by Drugs", **CURRENT MEDICINAL CHEMISTRY** *17*, 3514-3532

80. Agelis, G; Roumelioti, P; Resvani, A; **Durdagi, S**; Androutsou, ME; Kelaidonis, K; Vlahakos, D; Mavromoustakos, T; Matsoukas, J. **(2010)** "An Efficient Synthesis of a Rationally Designed 1,5 Disubstituted Imidazole AT(1) Angiotensin II Receptor Antagonist: Reorientation Of Imidazole Pharmacophore Groups in Losartan Reserves High Receptor Affinity And Confirms Docking Studies", **JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN** *24*, 749-758. DOI: 10.1007/s10822-010-9371-3

81. **Durdagi, S**; Papadopoulos, MG; Zoumpoulakis, PG; Koukoulitsa, C; Mavromoustakos, T, **(2010)** "A Computational Study on Cannabinoid Receptors and Potent Bioactive Cannabinoid Ligands: Homology Modeling, Docking, De Novo Drug Design and Molecular Dynamics Analysis" **Molecular Diversity** *14*, 257-276. DOI: 10.1007/s11030-009-9166-4

82. Innocenti, A; **Durdagi, S**; Doostdar, N; Strom, TA; Barron, AR; Supuran, CT. **(2010)** "Nanoscale Enzyme Inhibitors: Fullerenes Inhibit Carbonic Anhydrase by Occluding the Active Site Entrance", **BIOORGANIC & MEDICINAL CHEMISTRY** *18*, 2822-2828. DOI: 10.1016/j.bmc.2010.03.026

83. Fotakis, C; Gega, S; Siapi, E; Potamitis, C; Viras, K; Moutevelis-Minakakis, P; Kokotos, CG; **Durdagi, S**; Grdadolnik, SG; Sartori, B; Rappolt, M; Mavromoustakos, T. **(2010)** "Interactions at the Bilayer Interface and Receptor Site Induced by the Novel Synthetic Pyrrolidinone Analog MMK3", **BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES** 1798, 422-432, DOI: 10.1016/j.bbamem.2009.11.009

84. Politi, A; **Durdagi, S**; Moutevelis-Minakakis, P; Kokotos, G; Papadopoulos, MG; Mavromoustakos, T. **(2009)** "Application of 3D QSAR CoMFA/CoMSIA and in silico Docking Studies on Novel Renin Inhibitors Against Cardiovascular Diseases", **EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY** *44*, 3703-3711, DOI: 10.1016/j.ejmech.2009.03.040

85. **Durdagi, S**; Supuran, CT; Strom, TA; Doostdar, N; Kumar, MK; Barron, AR; Mavromoustakos, T; Papadopoulos, MG. **(2009)** "In Silico Drug Screening Approach for the Design of Magic Bullets: A Successful Example with Anti-HIV Fullerene Derivatized Amino Acids", **JOURNAL OF CHEMICAL INFORMATION AND MODELING** *49*, 1139-1143, DOI: 10.1021/ci900047s

86. Potamitis, C; Zervou, M; Katsiaras, V; Zoumpoulakis, P; **Durdagi, S**; Papadopoulos, MG; Hayes, JM; Grdadolnik, SG; Kyrikou, I; Argyropoulos, D; Vatougia, G; Mavromoustakos, T. **(2009)** "Antihypertensive Drug Valsartan in Solution and at the AT(1) Receptor: Conformational Analysis, Dynamic NMR Spectroscopy, in Silico Docking, and Molecular Dynamics Simulations", **JOURNAL OF CHEMICAL INFORMATION AND MODELING** *49*, 726-739. DOI: 10.1021/ci800427s

87. Kapou, A; Benetis, NP; **Durdagi, S**; Nikolaropoulos, S; Mavromoustakos, T. **(2008)** "3D QSAR/CoMFA and CoMSIA Studies on Antileukemic Steroidal Esters Coupled with Conformationally Flexible Nitrogen Mustards", **JOURNAL OF CHEMICAL INFORMATION AND MODELING** *48*, 2254-2264. DOI: 10.1021/ci800240m

88. **Durdagi, S**.; Mavromoustakos, T.; Chronakis, N.; Papadopoulos, M. G. **(2008)** "Computational Design of Novel Fullerene Derivatives as Potential HIV-1 PR Inhibitors: Analysis of Binding Interactions between Fullerene Inhibitors and HIV-1 PR Residues Using 3D QSAR, Molecular Docking and Molecular Dynamics Simulations" **BIOORGANIC & MEDICINAL CHEMISTRY** *16*, 9957-9974. DOI: 10.1016/j.bmc.2008.10.039

89. **Durdagi, S.,** Mavromoustakos, T. & Papadopoulos, M. G. **(2008)** "3D QSAR CoMFA/CoMSIA, Molecular Mocking and Molecular Dynamics Studies of Fullerene-based HIV-1 PR Inhibitors" **BIOORGANIC & MEDICINAL CHEMISTRY LETTERS** *18*, 6283-6289.

90. **Durdagi, S.,** Reis, H., Papadopoulos, M. G. & Mavromoustakos, T. **(2008)** "Comparative Molecular Dynamics Simulations of the Potent Synthetic Classical Cannabinoid Ligand AMG3 in Solution and at Binding Site of the CB1 and CB2 Receptors" **BIOORGANIC & MEDICINAL CHEMISTRY** *16*, 7377-7387.

91. **Durdagi, S.,** Papadopoulos, M. G., Papahatjis, D. P. & Mavromoustakos, T. **(2007)** "Combined 3D QSAR and Molecular Docking Studies to Reveal Novel Cannabinoid Ligands with Optimum Binding Activity" **BIOORGANIC & MEDICINAL CHEMISTRY LETTERS** *17*, 6754-6763.

92. **Durdagi, S**.; Kapou, A.; Kourouli, T.; Andreou, T.; Nikas, S. P.; Nahmias, V. R.; Papahatjis, D. P.; Papadopoulos, M. G.; Mavromoustakos, T. **(2007)** "The Application of 3D-QSAR Studies for Novel Cannabinoid Ligands Substituted at the C1' Position of the Alkyl Side Chain on the Structural Requirements for Binding to Cannabinoid Receptors CB1 and CB2" **JOURNAL OF MEDICINAL CHEMISTY** *50*, 2875-2885. DOI: 10.1021/jm0610705

93. Salzner, U; Karalti, O; **Durdagi, S. (2006)** "Does the Donor-Acceptor Concept Work for Designing Synthetic Metals? III. Theoretical Investigation of Copolymers Between Quinoid Acceptors and Aromatic Donors", **JOURNAL OF MOLECULAR MODELING** *12*, 687-701. DOI:10.1007/s00894-005-0046-2

94. **Durdagi, S**; Hofer, TS; Randolf, BR; Rode, B.M. **(2005)** "Structural and Dynamical Properties of Bi^{3+} in Water" **CHEMICAL PHYSICS LETTERS** *406*, 20-23. DOI: 10.1016/j.cplett.2005.02.082

(Total citations: ~1750; Average impact factor of published research papers and review articles: ~4.5; h-index: 25; * indicates corresponding author)

Patents

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

Published Abstracts, International Conference Proceedings

1. **Durdagi, S. 3rd Anticancer Drug Development Congress**. Molecular simulations of recently solved Co-crystallized X-ray structures clearly identifies action mechanism of PDEd inhibitors. **Turkey 2015.**

2. Gokdemir, E.; Mestanoglu, M.; Salmas, R.E.; **Durdagi, S. 3rd Anticancer Drug Development Congress.** Rehabilitating Drug-induced Long-QT Promoters-I: In-Silico Investigation of Action Mechanisms of Anti-Cancer Drugs with hERG1 K Channels and Oncogenic Targets. **Turkey 2015.**

3. Mestanoglu, M.; Gokdemir, E.; Salmas, R.E.; **Durdagi, S. 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.**

4. **Durdagi, S**.; 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**

5. **Durdagi, S.;** 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.***

6. **Durdagi, S. 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**.

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

8. **Durdagi, S**. **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**

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

10. Salmas, R.E.; **Durdagi, S**.; 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**

11. Zervou, M.; Cournia, C.; Potamitis, C.; Patargias, G.; **Durdagi, S**.; Grdadolnik S.G., Mavromoustakos, T. **247th ACS National Meeting and Exposition** "Molecular Basis of Action of the AT1 Antagonist Losartan" ***U.S.A.* 2014**

Published Abstracts, International Conference Proceedings (Cont.)

12. Noskov, S.Y.; **Durdagi, S**.; 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**.

13. **Durdagi, S.**; 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**.

14. **Durdagi, S**.; Randal, T.; Duff, H.J.; Noskov, S.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**.

15. Yazdi, S.; **Durdagi, S.**; 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**.

16. **Durdagi, S**.; 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**.

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

18. **Durdagi S.**; 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**.

19. **Durdagi, S**; 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**.

20. Agelis, G.; Resvani, A.; **Durdagi, S**.; Tumova, T.; Slaninov, J.; Giannopoulos, P.; Spyridaki, K.; Liapakis, G.; Vlahakos, D.; Mavromoustakos, T.; Matsoukas, J. **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.**

21. **Durdagi, S**; 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**.

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

23. **Durdagi, S. 3rd Kananaskis Symposium on Theoretical Models in Chemistry and Biology** "Recent Advances in Protein-Protein Docking algorithms" ***Canada*** **2011.**

24. Zoumpoulakis P., **Durdagi S**., 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**

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", 55, ***Turkey* 2007**

Published Abstracts, International Conference Proceedings (Cont.)

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**.

National Conference Proceedings

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 (Selected)

- **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.

Collaborations

Prof. Henry J Duff, University of Calgary, Faculty of Medicine, Calgary, AB, Canada

Prof. Philip Seeman, Toronto University, Canada

Prof. Aykut Uren, George Town University, Medical Center, USA

Prof. Mine Yurtsever, Istanbul Technical University, Department of Chemistry, Turkey

Prof. Sergei Y. Noskov, University of Calgary, Department of BioSciences, Calgary, AB, Canada

Prof. Thomas G Back, University of Calgary, Department of Chemistry, Calgary, AB, Canada

Prof. Thomas Mavromoustakos, University of Athens, Department of Chemistry, Athens, Greece

Prof. Manthos G. Papadopoulos The National Hellenic Research Foundation, Athens, Greece

Prof. Claudiu T Supuran, University of Florence, Department of Chemistry, Italy

Prof. Andrew R. Barron, Rice University, Department of Chemistry, USA

Prof. Deniz Ekinci, Max-Planck Institute of Molecular Cell Biology and Genetics, Germany

Prof. Murat Senturk, Agri Ibrahim Cecen University, Department of Chemistry, Turkey

Prof. Burak Erman, Koc University, Department of Chemical Engineering, Turkey

Prof. Matthias Stein, Max Planck Institute for Dynamics of Complex Technical Systems, Germany

Prof. Filiz Onat, Marmara University, School of Medicine, Turkey

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).