Kader Sahin, PhD.

School of Pharmacy, Bahçeşehir University, Istanbul, Turkey

E-mail: sahkader@hotmail.com, kader.sahin@med.bau.edu.tr

ACADEMIC

PostDoc: Computational Biology and Molecular Simulations Laboratory (Durdagi Research Group), Department of Biophysics, School of Medicine, Bahcesehir University, Istanbul, Turkey, January 2018 -2020

Ph.D.: Chemistry, Erciyes Univ (Turkey), August 2010

M.Sc.: Chemistry, Erciyes Univ (Turkey), June 2006

B.Sc.: Chemistry, Ankara Univ, Ankara,Turkey, February 2004

RESEARCH SUBJECTS

• Computer-Aided Drug Design

• Pharmacophore Modeling, 4D-QSAR (using EC-GA method (it was developed by our research group), PHASE

• Homology Modeling (using Rosetta-Membrane, Biopolymer Module of Sybyl etc.)

• Molecular Docking: Ligand-Protein and Protein-Protein Interactions (Glide, InducedFit, FlexX, AutoDock, GOLD, ClusPro)

• Molecular Dynamics Simulations (using CHARMM, GROMACS, NAMD, DESMOND, TRIPOS FF,etc.)

• De Novo Drug Design Applications (using CombIGlide, Leapfrog,etc.)

• Structure Elucidation, Conformational Analysis (using MM and QM methods)

• ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) Studies (using VolSurf)

• MM and QM Applications to Biological Systems (Gaussian 03/09, Schrodinger's Macro Model and Jaguar modules)

• De Novo Receptor and Loop modeling (using ROSETTA, YASARA programs)

• Programming-Code Development (ab initio pseudo potentials, local orbitals for ab initio molecular simulations)

Studied Systems

Anti-Cancer inhibitors (i.e., Inhibitory potencies of indole derivatives at BCL-2 enyzme: Molecular Docking, MD simulations, E-pharmacophore, Shape Base Screening applications were performed).

Anti-HIV inhibitors (i.e., Inhibitory potencies of indol derivatives at HIV-PR enyzme: Molecular Docking, MD simulations, 3D-QSAR, and De novo Drug Design applications were performed).

Coumarin Carboxamide Derivatives as eEF-2K Inhibitors (Homology modeling, Molecular Docking, MD simulations)

Identifying the Novel Pyrimidine-Based CDK2 Inhibitors: Molecular Docking, MD simulations

Anti-Hypertension inhibitors (i.e. Inhibitory potencies of indol derivatives at ACE enyzme: Molecular Docking, MD simulations, 3D-QSAR, and De novo Drug Design applications were performed).

Anti-Cancer inhibitors (i.e., Inhibitory potencies of piperazine derivatives at PARP-1 enyzme: Molecular Docking, MD simulations, 3D-QSAR, and De novo Drug Design applications were performed).

Carbonic Anhydrase (i.e. hCA-I, hCA-II, hCA-IX targets): Several ligands such as fullerenes, phenol derivatives, peptides were studied for their inhibitory profiles at these targets).

PUBLICATIONS

A. Published papers

1. Nuriye Dogan, Sevtap Cağlar Yavuz, **Kader Sahin**, Muge Didem Orhan, Hüseyin Kekec Muhammed, Seyma Calis,Fatma Öztürk Küp, Timucin Avsar,Senem Akkoc, Michael Tapera, Onur Sahin, Turker Kılıc, Serdar Durdagi, Emin Saripinar,Synthesis, Characterization, Biological Activity and Molecular Modeling Studies of Novel Aminoguanidine Derivatives, RSC Medicinal Chemistry (Submitted, 2022)

2. Michale Tapera, Hüseyin Kekeçmuhammed, **Kader Sahin**, Vagolu Siva Krishena, Christian Lherbet, Håvard Homberset, Tone Tønjum, Yunus Zorlu Serdar Durdagi, Emin Saripinar, Discovery of new compounds as Mycobacterium tuberculosis growth and enoyl acyl carrier protein reductase (InhA) inhibitors., Bioorganic Chemistry (submitted, 2022)

3. Ferah Comert Onder, **Kader Sahin**, Murat Sen turk, Serdar Durdagi, Mehmet Ay, Determination of highly effective coumarin compounds as cholinesterase inhibitors by in silico and in vitro studies. Journal of Molecular Graphics and Modelling, 2022, https://doi.org/10.1016/j.jmgm.2022.108210

4. **Kader Sahin**, Muge Didem Orhan, Timucin Avsar, Serdar Durdagi, Hybrid in Silico and TR-FRET-Guided Discovery of Novel BCL-2 Inhibitors, ACS Pharmacology & Translational, 2021, 4, 3, 1111–1123

5. **Kader Sahin**, Emin Sarıpınar, Serdar Durdagi, Combined 4D-QSAR and Target-based Approaches for the Determination of Bioactive Isatin Derivatives, SAR and QSAR in Environmental Research, 2021, 32,10, 769-792.

6. Serdar Durdagi, Cagdas Dag, Berna Dogan, Merve Yigin, Timucin Avsar, Cengizhan Buyukdag, Ismail Erol, Betul Ertem, Seyma Calis, Gunseli Yildirim, Muge D. Orhan, Omur Guven, Busecan Aksoydan, Ebru Destan, **Kader Sahin**, Sabri O. Besler, Lalehan Oktay, Alaleh Shafiei, Ilayda Tolu, Esra Ayan, Busra Yuksel, Ayse B. Peksen, Oktay Gocenler, Ali D. Yucel, Ozgur Can, Serena Ozabrahamyan, Alpsu Olkan, Ece Erdemoglu, Fulya Aksit, Gokhan Tanisali, Oleksandr M. Yefanov, Anton Barty, Alexandra Tolstikova, Gihan K. Ketawala, Sabine Botha, E. Han Dao, Brandon Hayes, Mengning Liang, Matthew H. Seaberg, Mark S. Hunter, Alex Batyuk, Valerio Mariani, Zhen Su, Frederic Poitevin, Chun Hong Yoon, Christopher Kupitz, Raymond G. Sierra, Edward Snell & Hasan DeMirci, Near-Physiological-Temperature Serial Femtosecond X-ray Crystallography Reveals Novel Conformations of SARS-CoV-2 Main Protease Active Site for Improved Drug Repurposing, Structures, 2021 Dec 2;29(12):1382-1396

7. Serdar Durdagi, Busecan Aksoydan, Berna Dogan, **Kader Sahin**, Aida Shahraki, Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of COVID-19 Main Protease: A Virtual Drug Re-Purposing Study, Mol. Inf. 2021, 40, 2100062, 1-14

8. **Kader Sahin**, In Silico identification of angiotensin-1 converting enzyme inhibitors using text mining and virtual screening, J. Biomol struct Dyn. (2020) DOI: 10.1080/07391102.2020.1827038

9. **Kader Sahin**, Investigation of novel indole-based HIV-1 protease inhibitors using virtual screening and text mining, J. Biomol struct Dyn. 2021, VOL. 39, NO. 10, 3638–3648

10. **Kader Sahin**, Emin Saripinar, A novel hybrid method named electron conformational genetic algorithm as a 4D QSAR investigation to calculate the biological activity of the tetrahydrodibenzazosines, Journal of Computational Chemistry, https://DOI:10.1002/jcc.26154, (2019)

11. **Kader Sahin**, Serdar Durdagi, Identifying New Piperazine-based PARP1 Inhibitors Using Text Mining and Integrated Molecular Modeling Approaches, J. Biomol struct Dyn, https://doi.org/10.1080/07391102.2020.1715262, (2019)

12. **Kader Sahin**, Serdar Durdagi, Identifying the Novel Pyrimidine-Based CDK2 Inhibitors as Anticancer Agents Using Text-Mining and Combined Molecular Modeling Approaches, JOTCSA. 2020;7(2):383–402.

13. **Kader Sahin**, Serdar Durdagi, Combined ligand and structure-based virtual screening approaches for identification of novel AChE inhibitors, Turkish Journal of Chemistry, (2020) 44: 574 – 588.

14. **Kader Sahin,** Belma Zengin Kurt, Fatih Sonmez, and Serdar Durdagi, Novel AChE and BChE inhibitors using combined virtual screening, text mining and in vitro binding assays, J. Biomol struct Dyn 2020, VOL. 38, NO. 11, 3342–3358.

15. Ferah Comert Onder, Serdar Durdagi, **Kader Sahin**, Bulent Ozpolat and Mehmet Ay, Design, Synthesis, eEF-2K Activity and Molecular Modeling Studies of Novel Coumarin Carboxamide Derivatives, Journal of Chemical Information and Modeling, https://doi.org/10.1021/acs.jcim.9b01083, (2019).

16. Seda Savranoglu Kulabas, Ferah Comert Onder, Yakup Berkay Yılmaz, Serdar Durdagi, **Kader Sahin**, Adem Ozleyen, Mehmet Ay, Tugba Boyunegmez Tumer, In vitro and in silico studies of nitrobenzamide derivatives as potential anti-neuroinflammatory agents, J. Biomol struct Dyn, doi.org https://doi.org/10.1080/07391102.2019.1684368, (2019)

17. Kuskucu, Akyildiz V, Kulmány Á, Ergün Yb Zencir S, Zupko I, Durdagi S, **Kader Sahin**, Zaka Me,Orhan H and Topcu Z, Structural modification of Ellipticine derivatives with alkyl groups of varying length is influential on their effects on human DNA topoisomerase II: A Combined Experimental and Computational Study, Medicinal Chemistry Research, DOI:10.1007/s00044-019-02472-9, (2019)

18. **Şahin K**., Sarıpınar E., Yanmaz E., Geçen N., Quantitative Bioactivity Prediction and Pharmacophore Identification for Benzotriazines Derivatives by Electron Conformational-Genetic Algorithm QSAR Method, SAR and QSAR in Enviramental Research, 22, 217-238 (2011)

19. Nazmiye Geçen, Emin Sarıpınar, Ersin Yanmaz, **Kader Sahin**, Application of Electron Conformational-Genetic Algorithm Approach To 1,4-Dihydropyridines as Calcium Channel Antagonists: Pharmacophore İdentification And Bioactivity Prediction, J Mol Model,18, 65-82 (2011)

20. Yanmaz E., Sarıpınar E., **Şahin K**., Geçen N., Çopur F., 4D-QSAR analysis and pharmacophore modeling: Electron conformational-genetic algorithm approach for penicillins, Bioorganic & Medicinal Chemistry, 19, 2199-2210, (2011)

21. E. Sarıpınar, N. Geçen, **K. Şahin**, E. Yanmaz, Pharmacophore Identification and Bioactivity Prediction for Triaminotriazine Derivatives by Electron Conformational-Genetic Algorithm QSAR Method, European Journal of Medicinal Chemistry, 45, 4157-4168, (2010).

PARTICIPATION IN FUNDED MULTI-DISCIPLINARY RESEARCH PROJECTS

1. Identification of Indole-based New Bioactive Molecules from Molecule Databases by Integration of Binary QSAR, Text Engineering and Combined Molecular Modeling Approaches, **Scholar, TUBİTAK 2218 Program**

2. Identification of Pharmacophore Showing Drug Effect, Investigation of Agonist and Antagonist Effects, and Bioactivity Calculation for Isatin Analogues, **Executive, TUBİTAK 3501**

3. Pharmacophore Identıfıcatıon and Bıoactıvıty Calculatıon for Benzyladenosine and Triaminotriazine, **Scholar, TUBİTAK 1001**

4. Pharmacophore Identıfıcatıon and Bıoactıvıty Calculatıon for Pyrazol, Benzotrıazın, Dıbenzazocıne and Quınazolıne Derıvatıves by Electron Conformatıonal-Genetıc Algorıthm 4D QSAR Method, **Scholar, Erciyes University**

INTERNATIONAL CONFERENCE PRESENTATIONS

1. **Kader Sahin**, Determination of pharmacophore group showing drug effect in isatin derivatives and bioactivity calculation, 7th International Bahcesehir University (BAU) Drug Design Congress, 19-21 Dec 2019, Istanbul, Turkey

2. **Kader Sahin**, Serdar Durdagi, Novel AChE and BChE Inhibitors Using Combined Virtual Screening, Text mining and In Vitro Binding Assays, 7th International Bahcesehir University (BAU) Drug Design Congress, 19-21 Dec 2019, Istanbul, Turkey

3. Emin Sarıpınar, Nazmiye Gecen, **Kader Sahin**, Ersin Yanmaz, Development of New Software in Drug Design and Application of Electron Conformational-Genetic Algorithm Method To 1,4- Dihydropyridine Derivatives, 18. Euro QSAR Symposium, 19-24 Sept 2010, Rhodes, Greece

4. Hayriye Yilmaz, Yahya Guzel, Nazmiye Gecen, **Kader Sahin** and M. Betul Aycan, 4D-QSAR Study Wıth Mcet Method on Estrogenic Activity Of 4,4-Dihydroxydifenylmethane as Bisfenola (Bsa) derivatives, 18. Euro QSAR Symposium, 19-24 Sept 2010, Rhodes, Greece

NATIONAL CONFERENCE PRESENTATIONS

1- **Kader Şahin**, Metin Madenciliği ve Kombine Moleküler Modelleme Yaklaşımlarını Kullanarak Yeni Piperazin Tabanlı PARP1 İnhibitörlerinin Belirlenmesi, 32. Ulusal Kimya Kongresi, 17-19 Eylül, 2020

2- **Kader Şahin**, QSAR İlkeleri ve Yapılmış Örnekler, Schrodinger Workshop, Biruni Üniversitesi, Eczacılık Fakültesi, 22 Mayıs, 2015

3- **Kader Şahin**, Emin Sarıpınar, Src Kinaz İnhibitörlerinin 4D QSAR Metodu ile Farmakofor Grubunun Belirlenmesi ve Biyoaktivite Hesabi, 24. Ulusal Kimya Kongresi-Zonguldak, 29 Haziran-2 Temmuz, 2010.

4- Emin Sarıpınar, Ersin Yanmaz, **Kader Şahin**, Nazmiye Geçen, İlaç Tasarımında Yeni Yazılımların Geliştirilmesi ve Elektron Konformasyonel-Genetik Algoritma Metodu, 24. Ulusal Kimya Kongresi-Zonguldak, 29 Haziran–2 Temmuz, 2010.

5- Nazmiye Geçen, **Kader Şahin**, Ersin Yanmaz, Fatih Çopur ve Emin Sarıpınar, İlaç Tasarımında Yeni Yazılımların Geliştirilmesi: Elektron Konformasyonel-Genetik Algoritma Metodu ile Triaminotriazin Bileşiklerinde Farmakofor Belirlenmesi ve Nicel Biyoaktivite Hesabı, I. Ulusal Yüksek Başarım ve Grid Konferansı, Orta Doğu Teknik Üniversitesi, Ankara, Nisan 2009

6- **Kader Şahin**, Nazmiye Geçen, Ersin Yanmaz, Fatih Çopur ve Emin Sarıpınar, Elektron Konformasyonel-Genetik Algoritma Metodu (EC-GA) ile Triaminotriazin Türevlerinde Farmakofor Belirlenmesi ve Nicel Biyoaktivite Hesabı, XXIII Ulusal Kimya Kongresi-Sivas, Haziran, 2009

Ph.D. THESIS

Pharmacophore Identification and Bioactivity Calculation for Pyrazol, Benzotriazin, Dibenzazocine and Quinazoline Derivatives by Electron Conformational-Genetic Algorithm 4D-QSAR Method was defended under supervision of Prof Emin Saripinar.

LABORATORY/COMPUTER SKILLS

Operating Systems: Linux, UNIX, Windows
Programming Languages: Pyhton, Matlab, Delphi, Java, C/C++, LaTeX

Application Programs/Softwares : SCHRODINGER Molecular Modeling package (Glide, IFD, Combiglide, Phase, Macromodel, Prime, Jaguar, etc.)**,** GAUSSIAN, SPARTAN, GAMES, GROMACS, TURBOMOLE, CASTEP, VASP, CHARMM, VolSurf (ADMET property prediction), SYBYL (3D QSAR/CoMFA, CoMSIA, FlexX Molecular Docking, Molecular Dynamics, LEAPFROG, MULTISEARCH, CONFORT (conformational search), MOLCAD, BIOPOLYMER, CLUSTERING, etc),GOLD Docking, Autodock, ClusPro, Scwrl, Rosetta-De Novo Modeling, CLUSTALW, BLAST, QUANTA/CHARMM,02, Origin, VMD, Molekel, HyperChem, ChemDraw, Pymol, VegaZZ, ChemPlus,etc.

CURRENT RESEARCH INTERESTS

• Molecular Docking and Molecular Dynamics Simulations

Study the binding interactions of drug molecules at the binding pocket of the receptor including membranes and design novel ligands that have optimized binding affinities, theoretically.

• 4D-QSAR Pharmacophore Modeling Studies and Conformational Analyses

Study of steric and electronic profiles of various classes of pharmaceutical molecules and rational design new lead compounds with improved properties.

• Abinitio and Semi-empirical Methods

Using abinitio and semi-empirical methods as well as application of other conformational analysis methodologies to explore the conformational space of drug molecules.

• Homology Modeling

Construction of homology models (i.e .by Rosetta-Membrane) to study the membrane protein structures.

Molecular Mechanism of the State-Dependant Drug Binding to the Ion Channels

Creation and validation of the molecular models describing the dynamics of activation and inactivation of ion channels.

Reviewer of the Journals

Journal of Enzyme Inhibition and Medicinal Chemistry

New Journal of chemistry

Journal of Biomolecular Structure and Dynamics

Anti-Cancer Agents in Medicinal Chemistry

Turkish Journal of Biology