Name / Surname: Kemal Yelekçi

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1. Education:

Degree	Major	University	Date
B.S.	Chemistry	Middle East Technical University	February 1979
M.S.	Organic Chemistry	Cukurova University	February 1981
Ph. D.	Organic Chemistry	Ohio University	March 1987
Post-doc	Organic-Medicinal Chemistry	Northwestern University (In Prof. Richard B. Silverman's group)	1987-1988

2. Career Objectives and Interest

Research and development involving studies of drug design and drug action, receptor ligand interaction and transporter protein mechanisms. *In silico* screening, calculation of free energy profile, elucidation of the flexibility and dynamical behavior of the protein-substrate complex are some of the major goals. To these aims our research group exploits computational techniques such as classical molecular dynamics (MD) simulations, quantum mechanics (QM), homology modeling and docking methods to investigate the structure, kinetics and thermodynamics of biological molecules, especially enzyme-ligand complexes. Applications of drug design tools to case studies are of special interest.

3. Selected Scientific Skills

- Considerable experience of *in silico* modelling.
- High-throughput screening of drug candidates.
- Experience in synthesis of biologically active compounds.
- Structure determination of organic compounds by spectroscopic methods (UV, IR, FT- NMR, 2D-NMR, MS etc.)
- Chromatographic separation methods (LC, GC, HPLC, GS-MS, etc.)
- Case study for Creating a three-dimensional *in silico* model of dopamine bound to the dopamine transporter with application to Parkinson's Disease.
- Extensive experience in molecular modeling for Histone Deacetylase (HDACs) and Histone Demethylase (LSD1).

4. Technical Skills

- Unix (Linux, MacOS) and Windows operating systems. MS-Office applications. Cluster experience.
- Experience in using Computer-aided drug design (CADD) packages:
 - Accelrys' Discovery Studio 4.5, (BIOVIA Foundation comprehensive predictive science application for the Life Sciences, more than 100 protocols).
 - NAMD (Nanoscale Molecular Dynamics) VMD (Visual Molecular Dynamics).
 - AutoDock 4.2 (Automated Docking Tools) and ADT (Autodock Tools).
 - Gaussian 10 and Gauss View

5. Grants and Projects:



TÜBİTAK-1003. 2015S009 "Development of Novel Synthetic Agents for Prostate Cancer Treatment." Researcher (2016-2020)



COST Action. (CM1406) "Epigenetic Chemical Biology (EPICHEM)". Member. (2015-2018)



FP7. Marie Curie Initial Training Networks (<u>ITN</u>). Call: FP7-PEOPLE-2013-ITN. Project ID: 608381. "Training in Neurodegeneration, Therapeutics Intervention & Neurorepair – TINTIN". Project member. (**2013-2017**)



İSTKA. "Establishment of Networking between Academia and Drug Companies and organization of a new Technology Center for a novel drug discovery, development and knowledge sharing- <u>İlaç Temel Araştırma Merkezi</u> – <u>İTAM</u>". Project member. (2012-2013)



COST Action CM1103. "Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain". Member. (2011-2015)



<u>TÜBİTAK-TBAG</u> 211T100. "In Silico Design of Selective Neuronal Nitric Oxide Synthase (nNOS) Inhibitors in Order to Prevent Neurodegenerative Diseases". Project Director. (2012-2013)



<u>TÜBİTAK</u> 1007 (105G01) . "Drug research and development for hereditary diseases caused by erroneous RNA splicing". Researcher (2006-2009)



FP6-MOBILITY. "Characterisation of Mitochondrial Proteins in Brain". Researcher. (2006-2010)



<u>TÜBİTAK-TBAG</u> 108T232 "Design of new pyrazoline derivatives using molecular modelling; synthesis and determination of their inhibition kinetics by computational and experimental techniques". Principal investigator. (2008-2010)



<u>TÜBİTAK-TBAG</u> 1332 194T033 "Ekmek Mayası (Saccharomyces Cerevisiae) Yardımı ile L-3,4-Dihidroksifenil Alanın (L-Dopa) için Yeni Bir Sentez Yöntemi". Principal investigator.(**2000-2004**)



<u>TÜBİTAK-TBAG 520</u> "Melia Azedarach L. (Tesbih ağacı) Meyvelerinin Özütlerinden İzole Edilen Etkin Maddeler ve Pamuk Zararlıları Üzerine Etkileri". Investigator. (1983-1986)

6. Recent Publications (last 5 years):

- 6.1 Kaan Birgül, Yeliz Yıldırım, H.Yeşim Karasulu, Ercüment Karasulu, Abdullah Ibrahim Uba, **Kemal Yelekçi**, Hatice Bekçi, Ahmet Cumaoğlu, Levent Kabasakal, Özgür Yılmaz, Ş.Güniz Küçükgüzel (2020). Synthesis, Anticancer Agents and Molecular Docking of (S)- Naproxen-1, 2, 4-Triazole Derivatives, *European Journal of Medicinal Chemistry*, 208.112841, **2020**. **IF: 5.572.** doi:10.1016/j.ejmech.2020.112841.
- 6.2 Özgür Yilmaz, Burak Bayer, Hatice Bekçi, Abdullah Ibrahim Uba, Ahmet Cumaoğlu, Kemal Yelekci, S Güniz Küçükgüzel (2020) Synthesis, Anticancer Activity on Prostate Cancer Cell Lines and Molecular Modeling Studies of Flurbiprofen-Thioether Derivatives as Potential Target of MetAP (type II). *Medicinal Chemistry*, 16(6), 735-749, 2020. doi:10.2174/1573406415666190613162322, PMID: 31203805, IF: 2.764.
- 6.3 Elmezayen, A. D., Al-Obaidi, A., Şahin, A. T., & Yelekçi, K. (2020). Drug repurposing for coronavirus (COVID-19): In silico screening of known drugs against coronavirus 3CL hydrolase and protease enzymes. *Journal of Biomolecular Structure and Dynamics*, 1-13. doi:10.1080/07391102.2020.1758791. IF: 3.107.
- 6.4 Elmezayen, A. D., & Yelekçi, K. (2020). Homology modeling and in silico design of novel and potential dual-acting inhibitors of human histone deacetylases HDAC5 and HDAC9 isozymes. *Journal of Biomolecular Structure and Dynamics*, doi:10.1080/07391102.2020.1798812, **IF:** 3.107.
- 6.5 Erensoy, G., Ding, K., Zhan, C. -., Elmezayen, A., Yelekçi, K., Duracik, M., . . . Küçükgüzel, İ. (2020). Synthesis, in silico studies and cytotoxicity evaluation of novel 1,3,4-oxadiazole derivatives designed as potential mPGES-1 inhibitors. *Journal of Research in Pharmacy*, 24(4), 436-451. doi:10.35333/jrp.2020.187.
- 6.6 Uba, A. I., & Yelekçi, K. (2020). Crystallographic structure versus homology model: A case study of molecular dynamics simulation of human and zebrafish histone deacetylase 10. *Journal of Biomolecular Structure and Dynamics*, 38(15), 4397-4406. doi:10.1080/07391102.2019.1691658. **IF: 3.107.**
- 6.7 Jackson Weako, Abdullahi Ibrahim Uba, Özlem Keskin, Attila Gürsoy, Kemal Yelekçi (2020). Identification of potential inhibitors of human methionine aminopeptidase (type II) for cancer therapy: structure-based virtual screening, ADMET prediction and molecular dynamics studies. *Computational Biology and Chemistry*, 86, 107244. https://doi.org/10.1016/j.compbiolchem.2020.107244.
- 6.8 Coşkun, G. P., Djikic, T., Kalaycı, S., Yelekçi, K., Şahin, F., & Güniz Küçükgüzel, Ş. (2019). Synthesis, molecular modelling and antibacterial activity against helicobacter pylori of novel diflunisal derivatives as urease enzyme inhibitors. *Letters in Drug Design and Discovery*, 16(4), 392-400. doi:10.2174/1570180815666180627130208.

- 6.9 Djikic, T., Martí, Y., Spyrakis, F., Lau, T., Benedetti, P., Davey, G., . . . Yelekci, K. (2019). Human dopamine transporter: The first implementation of a combined in silico/in vitro approach revealing the substrate and inhibitor specificities. *Journal of Biomolecular Structure and Dynamics*, 37(2), 291-306. doi:10.1080/07391102.2018.1426044.
- 6.10 Goksen, U. S., Sarigul, S., Bultinck, P., Herrebout, W., Dogan, I., Yelekci, K., . . . Gokhan Kelekci, N. (2019). Absolute configuration and biological profile of pyrazoline enantiomers as MAO inhibitory activity. *Chirality*, 31(1), 21-33. doi:10.1002/chir.23027.
- 6.11 Han, M. İ., Bekçi, H., Uba, A. I., Yıldırım, Y., Karasulu, E., Cumaoğlu, A., Yelekçi, K., . . . Küçükgüzel, Ş. G. (2019). Synthesis, molecular modeling, in vivo study, and anticancer activity of 1,2,4-triazole containing hydrazide—hydrazones derived from (S)-naproxen. *Archiv Der Pharmazie*, 352(6) doi:10.1002/ardp.201800365.
- 6.12 Ibrahim Uba, A., & Yelekçi, K. (2019). Homology modeling of human histone deacetylase 10 and design of potential selective inhibitors. *Journal of Biomolecular Structure and Dynamics*, 37(14), 3627-3636. doi:10.1080/07391102.2018.1521747.
- 6.13 Samorlu, A. S., Yelekçi, K., & Ibrahim Uba, A. (2019). The design of potent HIV-1 integrase inhibitors by a combined approach of structure-based virtual screening and molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, 37(17), 4644-4650. doi:10.1080/07391102.2018.1557559.
- 6.14 Uba, A. I., Weako, J., Keskin, Ö., Gürsoy, A., & Yelekçi, K. (2019). Examining the stability of binding modes of the co-crystallized inhibitors of human HDAC8 by molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, doi:10.1080/07391102.2019.1615989.
- 6.15 Abdullahi Ibrahim Uba, Kemal Yelekçi (2018). Identification of potential isoform- selective histone deacetylase inhibitors for cancer therapy: a combined approach of structure-based virtual screening, ADMET prediction and molecular dynamics simulation assay. *Journal of Biomolecular Structure and Dynamics*, 36:12, 3231- 3245. doi: http://doi.org/10.1080/07391102.2017.1384402. (IF: 3.107).
- 6.16 Abdullahi Ibrahim Uba, Kemal Yelekçi (2018). Carboxylic acid derivatives display potential selectivity for human histone deacetylase 6: structure-based virtual screening, molecular docking and dynamics simulation studies. *Computational Biology and Chemistry*, 75: 131-142. https://doi.org/10.1016/j.compbiolchem.2018.05.004. (IF: 1.412).
- 6.17 Göknil Coşkun, Teodora Djikic, Taha Hayal, Nezaket Türkel, Kemal Yelekçi, Fikrettin Şahin, Ş Küçükgüzel, "Synthesis, Molecular Docking and Anticancer Activity of Diflunisal Derivatives as Cyclooxygenase Enzyme Inhibitors, *Molecules* 2018, 23, 1969; **2018** doi:10.3390/molecules23081969, (**IF:3.09**).
- 6.18 Abdullahi Ibrahim Uba, Kemal Yelekçi (2018). Homology modeling of human histone deacetylase 10 and design of potential selective inhibitors. Journal of Biomolecular Structure and Dynamics, https://doi.org/10.1080/07391102.2018.1521747. (IF: 3.107).

- 6.19 Augustine S. Samorlu, Kemal Yelekçi, Abdullahi Ibrahim Uba. The design of potent HIV-1 integrase inhibitors by a combined approach of structure-based virtual screening and molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics.*, (2018) (IF: 3.107).
- 6.20 Umut Salgin Goksen, Sevgi Sarigul, Patrick Bultinck, Wouter Herrebout, Ilknur Dogan, Kemal Yelekci, Gulberk Ucar, Nesrin Gokhan Kelekci, Absolute configuration and biological profile of pyrazoline enantiomers as MAO inhibitory activity, Chirality, 23 November 2018. https://doi.org/10.1002/chir.23027, (IF:1.83).
- 6.21 Işıl Çoruh, Özge Çevik, Kemal Yelekçi, Teodora Djikic, Ş Güniz Küçükgüzel Synthesis, anticancer activity, and molecular modeling of etodolac-thioether derivatives as potent methionine aminopeptidase (type II) inhibitors *Archiv der Pharmazie*, 3-4, 351, **2018.** https://doi.org/10.1002/ardp.201700195 (IF:2.29).
- 6.22 Uba, A. I., & Yelekçi, K. (2018). Pharmacophore-based virtual screening for identification of potential selective inhibitors of human histone deacetylase 6. *Computational Biology and Chemistry*, 77, 318-330. doi:10.1016/j.compbiolchem.2018.10.016, (IF: 1.412).
- 6.23 Ibrahim Uba, A., & Yelekçi, K. (2019). Homology modeling of human histone deacetylase 10 and design of potential selective inhibitors. *Journal of Biomolecular Structure and Dynamics*, 37(14), 3627-3636. doi:10.1080/07391102.2018.1521747.
- 6.24 Samorlu, A. S., Yelekçi, K., & Ibrahim Uba, A. (2019). The design of potent HIV-1 integrase inhibitors by a combined approach of structure-based virtual screening and molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, 37(17), 4644-4650. doi:10.1080/07391102.2018.1557559.
- 6.25 Uba, A. I., Weako, J., Keskin, Ö., Gürsoy, A., & Yelekçi, K. (2019). Examining the stability of binding modes of the co-crystallized inhibitors of human HDAC8 by molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, doi:10.1080/07391102.2019.1615989.
- 6.26 S.T. Karadeniz, S.U. Akgul, Y. Ogret, H.S. Ciftci, A. Bayraktar, H. Bakkaloglu, Y. Caliskan, K. Yelekci, A. Turkmen, A.E. Aydin, F.S. Oguz, M. Carin, and F. Aydin, "Corrected Panel-Reactive Antibody Positivity Rates for Hypersensitized Patients in Turkish Population With Calculated Panel-Reactive Antibody Software", http://dx.doi.org/10.1016/j.transproceed.2017.01.032, Transplantation Proceedings, 49, 445e447 (2017).
- 6.27 Katarina Nikolic, Lazaros Mavridis, Teodora Djikic, Jelica Vucicevic, Danica Agbaba, Kemal Yelekci and John B. O. Mitchell, Computational approaches for multi-target drug design Drug Design for CNS Diseases: Screening Methodologies, Book Chapter, pp. 18-37, Ramsay, R. R., Di Giovanni, G., eds. (2017). Structure-Based Drug Design for Diagnosis and Treatment of Neurological Diseases. Lausanne: *Frontiers Media. doi: 10.3389/978-2-88945-123-4*.
- 6.28 Katarina Nikolic, Lazaros Mavridis, Teodora Djikic, Jelica Vucicevic, Danica Agbaba, KemalYelekci and John B. O. Mitchell. "Drug Design for CNS Diseases: Polypharmacological

- Profiling of Compounds Using Cheminformatic, 3D-QSAR and Virtual Screening Methodologies" http://dx.doi.org/10.3389/fnins.2016.00265. Front. Neurosci., (2016).
- 6.29 Evranos-Aksöz B, Baysal İ, Yabanoğlu-Çiftçi S, Djikic T, Yelekçi K, Uçar G, Ertan R. "Synthesis and Screening of Human Monoamine Oxidase-A Inhibitor Effect of New 2-Pyrazoline and Hydrazone Derivatives". *Arch Pharm (Weinheim)*. 2015 Oct;348(10):743-56. doi: 10.1002/ardp.201500212. Epub 2015 Aug 21. (2015).
- 6.30 F. Pinar Turkmenoglu, İpek Baysal, Samiye Ciftci-Yabanoglu, Kemal Yelekci, Hamdi Temel, Salih Paşa, Nurten Ezer, İhsan Çalış and Gulberk Ucar., "Flavonoids from Sideritis Species: Human Monoamine Oxidase (hMAO) Inhibitory Activities, Molecular Docking Studies and Crystal Structure of Xanthomicrol." *Molecules Journal*, 2015 Apr 23;20(5):7454-73. doi: 10.3390/molecules20057454. (2015).
- 6.31 Kemal Yelekci, Bahanur Örtmen., "De Novo Design of Potent and Selective Neuronal Nitric Oxide Synthase (nNOS) Inhibitors by a Fragment-Based Approach". *Journal of Pharmaceutical Chemistry*, ISSN: 2349-5731 (**2015**).
- 6.32 Malcomson T, Yelekci K, Mar Borrello MT, Ganesan A, Semina E, De Kimpe R, Mangelinckx S, Ramsay RR., "cis-Cyclopropylamines as mechanism-based inhibitors of Monoamine Oxidases", *FEBS Journal*, DOI: 10.1111/febs.13260, (2015).

7. International Conferences (last 5 years):

- 7.1 Yelekci, Kemal; Uba, Abdullahi "Intermolecular interactions in human HDAC8 crystal structures and the stability of binding modes of co-crystallized inhibitors", Conference: ACS Fall National Meeting and Exposition Location: San Diego, CA, USA. ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY Volume: 258 Meeting Abstract: 254 COMP Published: AUG 25 2019.
- 7.2 Kemal Yelekci, Abdullah İbrahim Uba, "The search for potential selective inhibitors of human histone deacetylase 6 via pharmacophore-based virtual screening". European Cooperation in Science and Technology (COST) Action CM1406: Epigenetic Chemical Biology ECI Workshop and Core Group Meeting, Institute Pasteur, 15th February, **2018**, Paris, FRANCE
- 7.3 Kemal Yelekçi, Abdullahi I. Uba, "In silico modeling of histon deacetyase enzyme and design of novel inhibitors Computational Chemistry: Application of Molecular Dynamics Simulation and Docking Approaches in Drug Design". Turkey, Epigenetic Chemical Biology Action CM1406 Computational Methods in Drug Design, 21.03.**2018.**
- 7.4 Kemal Yelekçi, "In silico identification of Isoform-Selective HDAC Inhibitors", EpiChemBio (CM1406) and MuTaLi COST (CA15135), Porto/ Portugal, September, **2017**.

- 7.5 Kemal Yelekçi, Abdullahi I. Uba, "Identification of HDAC6 selective inhibitors via structure-based virtual screening and molecular dynamics simulation assay", 5th International BAU Drug Design Congress, Istanbul, October, **2017**.
- 7.6 Kemal Yelekci, Teodora Djikic, "In silico Modeling of Dopamine Transporter and Design of Novel Neuroprotective Agents", 252nd ACS National Meeting in Philadelphia, PA, USA, August 21-25, p. 138, **2016**.
- 7.7 Yelekçi, K. ve Djikic, T. "In Silico Modeling of Human Dopamine Transporter and Design of Novel Inhibitors", 5st International Conference on Medicinal Chemistry, 01-03.07. **2015**, Avignon, France, p. 141.

Theses Advised:

Master of Science

- 1. Anas Abdulqader Abbas Al-Obaidi, "Development of Novel and Potent Inhibitors For GABA-AT Enzyme Via In Silico Screening Methods", **2020**.
- 2. Safanah Albayati. Master's Thesis. "Selective and Potent Inhibitors Design for Methionine Aminopeptidase II (MetAPs II) using Pharmacophore Modeling" (2019).
- 3. Şafak Naz Şentürk. Master's Thesis. "Peptidomimetic drug candidates for methionine amino peptidase II enzyme for prevention of cancer". (2019).
- 4. Augustine S. Samorlu. Master's Thesis. "In silico screening of potent HIV-1 integrase inhibitors for the treatment of human immunodeficiency virus (HIV)", (2018).
- 5. Sedat Tanju Karadeniz. Master's Thesis. "Corrected PRA positivity rates for hypersensitized patients in Turkish population with calculated PRA-cPRA software". (2017).
- 6. Jackson Weako. Master's Thesis. "In silico screening of tangible-potential inhibitor of methionine aminopeptidase 2 for the treatment of cancer", (2017).
- 7. Sinan Fındık. Master's Thesis. "Exploring the action mechanism of amphipathic alpha -Helical Antimicrobial Peptides, Ll-23 And Its Single-Nucleotide Variants Via Computational Methods", (2016).
- 8. Bahanur Örtmen. Master's Thesis. "In silico screening of neuronal nitric oxide synthase enzyme inhibitors" (2014).
- 9. Dilara Karaman. Master's Thesis. "In silico design and modeling of coumarin derivatives as selective monoamine oxidase A inhibitors", (2014).

- 10. Tuğba Mehmetoğu. Master's Thesis. "In silico design of novel and highly selective cyclooxygenase-2 inhibitors", (2014).
- 11. Talha Karabıyık. Master's Thesis. "In silico identification of physiological substrates and inhibitors of serum paraoxonase I enzyme", (2014).
- 12. Nurdan Kayrak. Master's Thesis. "nNOS selective inhibitor identification using de novo design methods", (2013).
- 13. Bora Büyüktürk. Master's Thesis. "Exploration of binding sites of nNOS isozymes to design selective neuronal nitric oxide synthase inhibitors", (2013).
- 14. Serkan Altuntaş. Master's Thesis. "In silico screening of monoamine oxidase A and B inhibitors using indane ring as a scaffolds", (2013).
- 15. Çağla Mıdık. Master's Thesis. "Monoamin oksidaz A ve B (MAO-A, MAO-B) enzimlerine ihnibitör olarak 1-tiocarbomoyil, 3-fenil, 5-furfuril, 2-pirazolin iskeleti kullanılarak daha aktif türevlerinin moleküler modelleme yöntemiyle tasarlanması", (2012).
- 16. Filiz Varnalı. Master's Thesis. "Monoamin oksidaz A ve B (MAO-A, MAO-B) enzimlerine inhibitör olarak 1-benzoksazilidinone-3,5-difenil-2-pirazolin iskeleti kullanılarak türevlerinin moleküler modelleme yöntemiyle tasarlanması", (2012).
- 17. Erçin Dinçer. Master's Thesis. "Tüberküloz (Mycobacterium Tuberculosis) bakterisinin LAM 7 suşunun rpoB geninin kodladığı rifambisin hedefini oluşturan proteinin homology modellenmesi ve mutasyona uğramış LAM 7 suşlarında oluşan dirence karşı yeni ilaç tasarımı", (2012).
- 18. Seyhan Türkkan. Master's Thesis. "Monoamin A ve Monoamin B enzimlerinine İnhibitör Tasarımı", (2012).
- 19. Özlem Karahan. Master's Thesis. "Monoamin oksidaz (MAO) enziminin aminleri oksitleme mekanizmasının hesapsal yöntemlerle incelenmesi", (2004).
- 20. İbrahim Yıldız. Master's Thesis. "Mono amin oksidaz (MAO) enziminin ekleme eliminasyon mekanizmasının hesapsal yöntemlerle incelenmesi", (2003).
- 21. Gül Altınbaş. Master's Thesis. "Benzen ve toluenin değişik substratlarla Friedel Crafts açilasyon reaksiyonlarının incelenmesi", (2001).
- 22. Dilber Damar. Master's Thesis. "Etil 2-nitro-3-hidroksi-3-(3,4-dimetoksifenil) propanoat'ın sentezi", (2001).
- 23. Memet Vezir Kahraman. Master's Thesis. "Synthesis of α -(2-aminomethyl)-N-phenyl nitrones", (1995).

Ph. D.

- 1. Sevim Karataş. PhD Thesis. "Synthesis of Ethyl alpha halo-3,4 disubstituted cinamate and alpha acyl-3,4- disubstituted cinamic acids and their reduced products with Pd/C, (2001).
- 2. Memet Vezir Kahraman. PhD Thesis. "Synthesis of biologically active amino ether synthesis", (2001).
- 3. Teodora Djikic "In silico reconstruction of the dopamine transporter and design of new drugs with neuroprotective properties", 2017.
- 4. Abdullahi İbrahim Uba, "*In silico* Design of Novel Epigenetics-based Anticancer agents via Histone Deacetylase Inhibition", 2018.
- 5. Ammar Almezayan, "In Silico Designing of Isoform-Selective Inhibitors Against Class IIa Histone Deacetylases", 2021.
- 6. Sedat Tanju Karadeniz, "Augmented Virtual-Cross-Match for Donor-Induced Antibody Prediction by Using High Resolution HLA Typing and HLA Epitope Mapping for Better Donor Match", 2021
- 7. Sarah Boumezber, "Designing of Selective and Potential of Neuronal Nitric Oxide Synthase Inhibitors Toward the Prevention Neurodegenerative Disease Using in Silico Screening Methods", 2021.

Awards:

- The academic award of 2014. (Given by Kadir Has University to the best academic staff whose achievement in research and teaching are commendable)
- Novartis Award for Drug Design, Turkey (2008)
- Kadir Has University, Award of Education and Research (5 times)
- DAAD Scholarship (For German education at Goethe Institute)
- Fulbright Scholarship (For PhD education at Ohio University)
- NATO Grant (Collaborative Research with Prof. Richard B. Silverman at Northwestern University, 1995-1997)
- NIH (National Institutes of Health) Post-doctorate grant (with Prof. Richard B. Silverman at Northwestern University, 1986-1988).

Membership:

- Turkish Chemical Society
- American Chemical Society (ACS)
- METU İstanbul Grads' Association

Administrative Duties

- Kadir Has University, Department Head of Bioinformatics and Genetics (2008 now)
- Kadir Has University, Dean of Faculty of Science and Letters (2001-2006)
- Kadir Has University, Vice Rector (2001-2003)
- Marmara University, Dean of Faculty of Science and Letters (1998-2001)
- Marmara University, Department Head of Organic Chemistry (1994-2000)
- Marmara University, Department Head of Chemistry (1988-2000)

Courses offered:

Undergraduate:

- General Chemistry
- Organic Chemistry
- Introduction to Spectroscopy
- Nuclear Magnetic Resonance Spectroscopy
- Instrumental Analysis
- Introduction to Stereochemistry

Graduate:

- Introduction to Bioinformatics
- Organic Chemistry of Drug Design and Drug Action
- Special Topics in Medicinal Chemistry
- Introduction to Nuclear Magnetic Resonance (NMR)
- Advanced Nuclear Magnetic Resonance Spectroscopy (NMR)