Semiha Kevser Bali

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I am a computational chemist with experience in applying various molecular modeling and cheminformatics techniques on drug discovery projects as well as understanding environmental pollutants. Currently seeking my next step in the drug discovery field where I can utilize my expertise in collaborative academic and industry settings.

Education

Michigan State University — East Lansing, MI
Ph.D., Chemistry, Advisor: Dr. Angela K. Wilson — *2019 - 2024(expected)*

Bogazici University — Istanbul, Turkey
M.Sc., Chemistry. Thesis title: Activity of Topotecan as Topoisomerase IB Inhibitor — *2016 – 2018*

Bogazici University — Istanbul, Turkey
B.S., Molecular Biology & Genetics — *2010 – 2015*

Research Experience

Co-op at Moderna — Jan. 2022 - June 2022
Molecular Engineering and Modeling Group — *Cambridge, MA*

- Created a workflow that models RNA-small molecules to effectively screen synthesized small compounds based on their affinity towards certain types of RNA tertiary structures. Tested available methods to assess their performance to be used for our target systems. Investigated bilayer interactions with various lipids and their binding through metadynamics studies.

Ph.D. Candidate at Michigan State University — Aug. 2019 - current
Department of Chemistry, Wilson Research Group — *East Lansing, MI*

- Collaborated with medicinal chemists and microbiologists to create novel compounds to be used against Tuberculosis by utilizing various computational tools, and understanding the mechanism of actions.
- Modeled the toxic effects of per and poly-fluoroalkyl substances (PFAS) on selected human and fish proteins to understand the molecular details of the PFAS-protein interactions, suggest experimental partners potential protein targets to focus on, and to develop mitigation strategies. By combining molecular modeling and AI, designing novel, less toxic PFAS alternatives.
- Provided computational chemistry support for Reata Pharmaceuticals on their drug discovery programs.
- Successfully taught and mentored three undergraduate students and trained newly accepted graduate students.
- Teaching assistant for three semesters for the General Chemistry Laboratory course and molecular biology seminar course for one semester.

Graduate Student Researcher at Universite de Lorraine — Feb. 2019 - July 2019
Laboratoire de Physique et Chimie Théoriques (LPCT) — *Nancy, France*

- Investigated the aggregation of amyloid-beta peptides in different biological lipid bilayer compositions using coarse-grained and atomistic molecular dynamics simulations, by collaborating with experimentalists. This work is published under the guidance of Prof. Mounir Tarek.

Master's Degree at Bogazici University — Jan. 2016 - July. 2018
Department of Chemistry — *Istanbul, Turkey*

- Investigated the activity difference between two forms of Topotecan drug molecule using Molecular Dynamics and hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) approaches for my Master's thesis. Thesis advisors: Prof. Viktorya Aviyente, Prof. Saron Catak.
- Uncovered the DNA base selectivity of two different families of cancer drugs that target TopoIB using Molecular Dynamics and hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) approaches.
- Modeled Diel-Alder reactions using quantum mechanical methods (QM), in collaboration with organic chemists.

Short-term Visiting Researcher at Michigan State University — Aug. 2018 - Dec. 2018
Department of Chemistry — *East Lansing, MI*

- Parametrized the interaction between calcium and phosphate groups using LJ 12-6-4 method for accurately modeling dental adhesives synthesized by our experimental collaborators. Supervised by Prof. Kenneth Merz Jr.

Undergraduate Research Intern at Bogazici University June 2014 - Dec. 2015

Department of Chemistry *Istanbul, Turkey*

- Modeled the iron release mechanism from the N-lobe of human Transferrin protein using quantum mechanical (DFT) calculations. Supervised by Profs. Viktorya Aviyente & Burcu Dedeoglu. This work is published.

Technical Skills

- Classical Molecular Dynamics (MD) simulations with Amber, Gromacs, NAMD
- Umbrella Sampling and Steered Molecular Dynamics simulations
- Alchemical Binding Free Energy calculations with Thermodynamic Integration (TI)
- Hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) calculatins
- Quantum mechanical (QM) calculations for protein active site modeling and reaction modeling
- Programming with Python, scripting with Bash and LaTeX

Journal Publications

1. **Bali, S. K.**[*]; Haslak, Z. P.; Cifci, G.; Aviyente, V. DNA Selectivity of Indenoisoquinolines: A Computational Approach. *Org. Biomol. Chem.* , **2023**, 21, *4518-4528*. [*]corresponding author.
2. Siniscalco, D.; Francius, G.; Tarek, M.; **Bali, S. K.**; Malaplate, C.; Oster, T.; Pauron, L.; Quilès, F. Molecular Insights for Alzheimer's Disease: an Unexplored Storyline on the Nanoscale Impact of Nascent Aβ1-42 towards Lipid Membrane. *ACS Appl. Mater. Interfaces*, **2023**,*15(14)* 17507–17517.
3. Findik, B. K.; Cilesiz, U.; **Bali, S. K.**; Atilgan, C.; Aviyente, V.; Dedeoglu, B. Investigation of Iron Release from the N- and C- Lobes of Human Serum Transferrin by Quantum Chemical Calculations *Org. Biomol. Chem.*, **2022**, *20*, 8766-8774.
4. **Bali, S. K.**; Marion, A.; Ugur, I.; Dikmenli, A. K.; Catak, S.; Aviyente, V. Activity of Topotecan toward the DNA/Topoisomerase I Complex: A Theoretical Rationalization. *Biochemistry*, **2018**, *57*(9), 1542-1551.
5. Kilic, H.; Bayindir, S.; Erdogan, E.; Agopcan Cinar, S.; Konuklar, F. A. S.; **Bali, S. K.**; Saracoglu, N.; Aviyente, V. Bismuth nitrate-promoted disproportionative condensation of indoles with cyclohexanone: a new-type azafulvenium reactivity of indole. *New J. Chem.*. **2017**, *41*(18), 9674-9687.
6. Almeida, N. M. S.[+] and **Bali, S. K.**[+]; James, D.; Wang, C.; Wilson, A. K. Binding of per- and polyfluoroalkyl substances (PFAS) to the PPARg/RXRa-DNA complex. *Manuscript submitted.* [+]co-authors
7. **Bali, S. K.**, Martin,R.; Almeida, N. M. S.; Saunders, C.; Wilson, A. K. The effect of selected PFAS compounds on human Thyroglobulin protein. *Manuscript in preparation.*
8. **Bali, S. K.**, Hall,K.; Almeida, N. M. S.; Massoud, R.; Wilson, A. K. Understanding PFAS toxicity for Estrogen Receptors in fish from the Great Lakes. *Manuscript in preparation.*

Conference Presentations

1. **Bali, S. K.**; Almeida, N. M. S.; James, D.; Wang, C.; Martin, R.; Hall, K.; Nair, A.; Wilson, A. K. "Understanding PFAS toxicity through computational approaches". **Invited Oral** presentation, ACS CERM 2023 Meeting, Detroit, MI, June 20—23, 2023.
2. **Bali, S. K.**; Wilson, A. K. "Addressing Global Health and Environmental Challenges with Computational Chemistry". **Poster** presentation, Schrodinger Catalyzing Gender Equity, New York City, NY, May 23—24, 2023.
3. **Bali, S. K.**; Almeida, N. M. S.; James, D.; Nair, A.; Wilson, A. K. "PFASs: Computational study on their impact on PPARg-RXRa heterodimer". **Oral** presentation, ACS 2023 Spring National Meeting, Indianapolis, IN, March 26—30, 2023.
4. **Bali, S. K.**; Almeida, N. M. S.; James, D.; Nair, A.; Wilson, A. K. "The Effect of PFAS on PPAR-gamma/RXR-alpha Heterodimer." **Oral** presentation, 67th Biophysical Society Annual Meeting, San Diego, CA, Feb.18—22, 2023.
5. **Bali, S. K.**; Almeida, N. M.S.; James, D.; Nair, A.; Martin, R.; Saunders, C.; Wilson, A. K. **Poster** presentation, Inaugural Annual Symposium on Emerging Technologies in PFAS Remediation and Toxicity, East Lansing, MI, Oct. 25, 2022.
6. **Bali, S. K.**; Saunders, C.; Martin, R.; Almeida, N. M. S.; Wilson, A. K. "Effect of PFAS on human Thyroglobulin Protein: An in-silico approach". **Poster** presentation, 52nd Midwest Theoretical Chemistry Conference, Columbus, OH, June 2—4, 2022. *Selected as an honorable mention.*

7. **Bali, S. K.**; Saunders, C.; Martin, R.; Almeida, N. M. S.; Wilson, A. K. "Effect of PFAS compounds: an in silico approach". **Poster** presentation, ACS 2022 Spring National Meeting, San Diego, CA, March 20—24, 2022.
8. **Bali, S. K.**; Marion, A.; Ugur, I.; Dikmenli, A. K.; Catak, S.; Aviyente V. "Rationalization of the activity of the lactone form of topotecan towards the DNA/topoI complex". **Poster** presentation, Chemistry ViA Computation, Istanbul, Turkey, October 30, 2017.
9. **Bali, S. K.**; Marion, A.; Ugur, I.; Dikmenli, A. K.; Catak, S.; Aviyente V. "Anti Kanser İlacı Topotecan'ın Karboksilat ve Lakton Formlarının Bağlanma Mekanizmasının Aydınlatılması". **Poster** presentation, 29th National Chemistry Congress, Ankara, Turkey, September 10—14, 2017.
10. **Bali, S. K.**; Marion, A.; Ugur, I.; Catak, S.; Aviyente V. **Poster** presentation, 3rd Workshop on High-Throughput Molecular Dynamics (HTMD), Barcelona, Spain, November 10—11, 2016.

Extracurricular Activities

- Served as Chemistry Dept representative in the Council of Graduate Students (COGS) in 2022-23, a university-recognized student government body. Organizing member of the Graduate Academic Conference in 2023
- Elect-secretary of Council of Graduate Students (COGS) for 2023-24.
- Founding member and serving as a Senator in Chemistry Graduate Student Organization in 2022-23.
- Founding member and vice-president of Michigan State University Biophysical Student Chapter in 2023-24.

Honors and Awards

- Outstanding Scholar Fellowship, Collage of Natural Sciences — Ph.D. Candidate
- TUBITAK 1001 Project Student, Grant No: 215Z399 — Master's Degree
- Sabanci Foundation, University Admission Scholarship — Bachelor's Degree

References

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