Mehmet Aziz Yirik

Faculty of Pharmacy
Bahcesehir University, Istanbul, Turkiye

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PERSONAL

Date of Birth: March 30, 1991
Place of Birth:Istanbul,Turkiye
Citizenship: Turkish

EDUCATION

Friedrich-Schiller-University Jena
PhD Candidate – Mathematical and Algorithmic Cheminformatics
September 2017 – May 2022
Thesis: Development of Chemical Graph Generators (supervisor: Christoph Steinbeck)

Bogazici University, Istanbul, Turkiye
MA in Computational Science and Engineering
February 2014 – August 2017
Thesis: Development of a Data Collection and Analysis Tool for Protein-Ligand Interactions

Mimar Sinan University, Istanbul, Turkiye
BA in Mathematics
2009 - 2013
Project 1: Special Topics in Partial Differential Equations (supervisor: Muge Meyvaci)
Project 2: Group Theory and Symmetry (supervisor: Ayse Berkman)

EMPLOYMENT

Assistant Professor in Computational Drug Design

Faculty of Pharmacy
October 2025 – Present

Postdoctoral Researcher - EU Horizon Project

IMADA, University of Southern Denmark
June 2022 – May 2025

Scientific Researcher and Teaching Assistant

Friedrich-Schiller-University Jena, Germany
September 2017 – December 2021

Research Project Assistant

Bogazici University, Istanbul,Turkiye
November 2016 – June 2017
Project was funded by the Scientific and Technological Research Council of Turkiye

Lecturer

Mimar Sinan University, Istanbul, Turkiye
February – June 2016
Course Name: Graph Theory and Its Applications in Computational Biology

PUBLICATIONS

- Yirik M.A., Andersen J.L., Fagerberg R., Merkle D. ChemReservoir - An Open-Source Framework for Chemically-Inspired Reservoir Computing, IEEE Access, vol. 13, pp. 149197-149202, 2025, https://doi.org/10.1109/ACCESS.2025.3602358
- Ekim T, Shalom M, Yirik MA. Generation of weighted trees, block trees and block graphs. arXiv preprint arXiv:2401.09764. 2024 Jan 18. https://doi.org/10.48550/arXiv.2401.09764
- Yirik, M.A., Sorokina, M. & Steinbeck, C. MAYGEN: an open-source chemical structure generator for constitutional isomers based on the orderly generation principle. *J Cheminform* **13,** 48 (2021). https://doi.org/10.1186/s13321-021-00529-9
- Yirik MA, Steinbeck C (2021) Chemical graph generators. PLoS Comput Biol 17(1): e1008504. https://doi.org/10.1371/journal.pcbi.1008504
- Sorokina, M., Merseburger, P., Rajan, K. *et al.* COCONUT online: Collection of Open Natural Products database. *J Cheminform* **13,** 2 (2021). https://doi.org/10.1186/s13321-020-00478-9
- Preprint/Chemical Graph Theory. (2022, May 1). Wikiversity. Retrieved 09:52, May 1, 2022 from https://en.wikiversity.org/w/index.php?title=Preprint/Chemical_Graph_Theory&oldid=2391985.
- Mayer-Bacon, C., Yirik, M. A. Curation of Computational Chemical Libraries Demonstrated with alpha-Amino Acids. *J. Vis. Exp.* (182), e63632, doi:10.3791/63632 (2022)
- McKay, B.D., Yirik, M.A. & Steinbeck, C. Surge: a fast open-source chemical graph generator. J Cheminform 14, 24 (2022). https://doi.org/10.1186/s13321-022-00604-9

PROJECTS

- "Complex chemical reaction networks for breakthrough scalable reservoir computing (CORENET) - EU Horizon Project" -SDU - Postdoctoral project: I have been working on the development of in-silico chemical reservoir models as a part of CORENET project.

- "Development of Efficient Open-Source Molecular Structure Generators" – FSU Jena – PhD Project: As the implementation of computational group theory and graph algorithms, I worked on the orderly graph generation problem for the development of open-source chemical graph generator. The method can be implemented in many other fields besides cheminformatics.

- "Development of a Data Collection and Analysis Tool for Protein-Ligand Interactions" – Bogazici University - Master Thesis: Development of data retrieval tool. Although the project focused on protein-ligand data, it provided valuable insights into database structures and the broader field of data analysis.

- "Calculating symmetry groups of Platonic and Archimedean Solids" - Mimar Sinan University - Bachelor Project: This project served as the initial step in understanding symmetry groups, which are applicable not only to molecular symmetry but also to a wide range of symmetrical objects.

- "Understanding Partial Differential Equations" – Mimar Sinan University – Bachelor project.

CONFERENCES AND PRESENTATIONS

- The Winter School of Computational Neuroscience, American University of Beirut (2016), Lebanon
- The Fourth BAU Drug Design Conference – Poster Presentation (2016), Istanbul/Turkiye
- de.NBI Winter School on Computational Metabolomics (2018), Wittenberg/Germany
- MATH/CHEM/COMP Conference – Poster Presentation (2019), Dubrovnik/Croatia
- MATH/CHEM/COMP Conference – Oral Presentation (2021), Dubrovnik/Croatia
- Cambridge Cheminformatics Meeting – Oral Presentation (2021) Cambridge, UK, (Virtual) https://www.youtube.com/watch?v=TGiqaZnZRgw
- ML4Molecules Workshop - Poster Presentation (2024), Fritz Haber Institute of the Max Planck Society, Berlin/Germany
- COMPASS Symposium - Oral Presentation (2025), Hanse-Wissenschaftskolleg Institute, Germany

RESEARCH INTERESTS

- Chemical Graph Theory
- Combinatorial Algorithms
- Algorithmic Cheminformatics
- Algorithmic Graph Theory

SKILLS

Languages

- Turkish - Native Language
- English - Professional Level
- German - B1 Level

REFERENCES

- Christoph Steinbeck, Friedrich Schiller University Jena, contact: christoph.steinbeck@uni-jena.de
- Ali Taheri, The University of Sussex, contact: A.Taheri@sussex.ac.uk
- Muge Meyvaci, Mimar Sinan University, contact: mmeyveci@msgsu.edu.tr
- Ayse Berkman, Mimar Sinan University, contact: ayse.berkman@msgsu.edu.tr

More references available upon request