

# Mehmet Aziz Yirik

Institute for Analytical Chemistry

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## PERSONAL

**Date of Birth:** March 30, 1991

**Place of Birth:** Istanbul, Turkey

**Citizenship:** Turkish

## EDUCATION

### Friedrich-Schiller-University Jena

PhD Candidate – Mathematical and Algorithmic Cheminformatics

September 2017 – December 2021

Thesis: Development of Chemical Graph Generator (supervisor: Christoph Steinbeck)

### Bogazici University, Istanbul, Turkey

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, Turkey

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

### Scientific Researcher and Teaching Assistant

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

### Research Project Assistant

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

### Teaching Assistant

Bogazici University, Istanbul, Turkey  
October 2016 – January 2017  
Course Name: “Protein Interactions: Molecules to Networks”

### Lecturer

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

## PUBLICATIONS

- 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>
- Yirik, M.A.; Colpan, K.E.; Schmidt, S.; Sorokina, M.; Steinbeck, C., Review on Chemical Graph Theory and Its Application in Computer-Assisted Structure Elucidation. *Preprints* **2021**, 2021110546 (doi: 10.20944/preprints202111.0546.v1).
- Mayer-B., C., Yirik, M.A., Methods for Curation of Computational Chemical Libraries, as demonstrated with alpha-Amino Acids, *Journal of Visualized Experiments*, 2021, (submitted)
- McKay BD, Yirik MA, Steinbeck C. Surge - A Fast Open-Source Chemical Graph Generator . *ChemRxiv*. Cambridge: Cambridge Open Engage; 2021; This content is a preprint and has not been peer-reviewed.

## PROJECTS

- “Development of Efficient Open-Source Molecular Structure Generators” – FSU Jena – Current PhD Project: As the implementation of computational group theory and graph algorithms, I have been working on 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 and application of improved cheminformatics methods for biosciences”, DAAD project: I contribute with my mathematics and cheminformatics knowledge to the development of new cheminformatics tools for this DAAD project between Germany-Croatia.
- “Development of a Data Collection and Analysis Tool for Protein-Ligand Interactions” – Bogazici University, Istanbul (2017): Although I worked on protein-ligand data, this project helped me to understand database structures and the data analysis in general.
- “Calculating symmetry groups of Platonic and Archimedean Solids” - Mimar Sinan University, Istanbul (2013): This project topic was the first step to understand symmetry groups which are also applicable for molecular symmetry and many other symmetric objects.
- “Understanding Partial Differential Equations” – Mimar Sinan University (2012)

## 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/Turkey
- 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=TGiqZnZRgw>

## RESEARCH INTERESTS

- Combinatorial Algorithms
- Graph Generators & Isomorphism
- Computational Group Theory
- Algorithmic Bio-Cheminformatics

## **SKILLS**

### **Languages**

- Turkish - Native Language
- English - (IELTS score: 6.5)
- German – B2 Level
- Arabic - Conversational

### **Computer Skills**

- Python
- JAVA
- MATLAB
- Cloud Computing - GCP

## **REFERENCES**

- Christoph Steinbeck, Friedrich Schiller University Jena, contact: [christoph.steinbeck@uni-jena.de](mailto:christoph.steinbeck@uni-jena.de)
- Ali Taheri, The University of Sussex, contact: [A.Taheri@sussex.ac.uk](mailto:A.Taheri@sussex.ac.uk)
- Muge Meyvaci, Mimar Sinan University, contact: [mmeyveci@msgsu.edu.tr](mailto:mmeyveci@msgsu.edu.tr)

More references available upon request