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 Virtual Experiments, 2021, (Submitted)
- McKay, B.D., Yirik, M.A., Steinbeck, C., surge - A Fast Chemical Graph Generator, (submitted). https://structuregenerator.github.io

PROJECTS

- "Development of Efficient Open-Source Molecular Structure Generators" – FSU Jena – Current PhD Project: As the implementation of computational group theory, I have been working on orderly graph generation problem for the development of open-source molecular structure generators. The method can be implemented in many other fields.

- "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 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)

RESEARCH INTERESTS

- Combinatorial Algorithms
- Graph Generators
- 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

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

More references available upon request