

Rıza Özçelik | Ph.D. candidate

✉ r.ozcelik@tue.nl • 🌐 rizaozcelik.github.io

Education

- 2022–2026: **Ph.D., Biomedical Engineering**, Eindhoven University of Technology, The Netherlands.
Thesis: Advancing Chemical Language Models for *De Novo* Drug Design
Supervisor: Francesca Grisoni
- 2018–2021: **M.Sc., Computer Engineering**, Boğaziçi University, Turkey.
GPA: 3.94/4.00 (High Honor). Thesis: Biomolecular Language Processing for Drug-Target Affinity Prediction
Supervisor: Arzucan Özgür and Elif Ozkirimli (Roche)
- 2014–2018: **B.Sc., Computer Engineering**, Boğaziçi University, Turkey.
GPA: 3.57/4.00 (High Honor). Thesis: Disease Classification based on Genomic Data with Machine Learning
Supervisor: Arzucan Özgür

Employment

- 06.2021 – 12.2021: **Great Minds Research Intern**, IBM Research, Zurich.
Translated natural language prompts to application pipelines. Implemented from scratch.
- 02.2019 – 12.2021: **Teaching Assistant**, Dept. of Computer Engineering, Boğaziçi University, Istanbul.
Taught lectures for more than 200 hours. More than 15% of written feedback called me "the best TA ever."
- 12.2018 – 06.2019: **Research Assistant**, Scientific Council of Turkey (TUBITAK), Istanbul.
Added modules to the open-source Turkish language processing library, nlptoolkit, as a core developer.
- 07.2018 – 12.2018: **Data Scientist**, ING Turkey, Istanbul.
Formulated cash flow management as a machine learning problem. Implemented solutions.

Publications

* Shared first authorship

- Özçelik, Rıza**, Sarah de Ruiter, Emanuele Cruscio, and Francesca Grisoni. "Chemical Language Modeling with Structured State Space Sequence Models." *Nature Communications*, 2024.
- Özçelik, Rıza**, and Francesca Grisoni. "A Hitchhiker's Guide to Deep Chemical Language Processing for Bioactivity Prediction." *arxiv preprint doi: 10.48550/arXiv.2407.12152*, 2024.
- Özçelik, Rıza**, Laura van Weesep, Sarah de Ruiter, and Francesca Grisoni. "peptidy: A Light-weight Python Library for Peptide Representation in Machine Learning." *ChemRxiv doi: 10.26434/chemrxiv-2024-bm3lv*, 2024.
- Birolo, Rebecca, **Rıza Özçelik**, Andrea Aramini, Roberto Gobetto, Michele R. Chierotti, Francesca Grisoni. "Leveraging Deep Chemical Language Processing for Co-crystal Prediction." *ChemRxiv doi: 10.26434/chemrxiv-2024-vgvhk*, 2024.
- van Tilborg, Derek, Helena Brinkmann, Emanuele Criscuolo, Luke Rossen, **Rıza Özçelik***, and Francesca Grisoni. "Deep learning for Low-data Drug Discovery: Hurdles and Opportunities." *Current Opinion in Structural Biology*, 2024.
- Büşra Temizer, Asu, Gökçe Uludoğan, **Rıza Özçelik***, Taha Koulani, Elif Ozkirimli, Kutlu Ulgen, Nilgun Karalı, and Arzucan Özgür. "Exploring Data-Driven Chemical SMILES Tokenization Approaches to Identify Key Protein-Ligand Binding Moieties." *Molecular Informatics*, 2024.
- Özçelik, Rıza**, Francesca Grisoni. "A Novel Evaluation Framework for De Novo Drug Design with Deep Learning." *In preparation*, 2024.
- van Weesep, Laura, **Rıza Özçelik***, Marloes Pennings, Luc Brunsveld, Francesca Grisoni. "Deep Learning for 14-3-3 Protein-Protein Interaction Prediction." *In preparation*, 2024.

9. **Özçelik, Rıza***, Derek van Tilborg, Jose Jiménez-Luna, and Francesca Grisoni. "Structure-based Drug Discovery with Deep Learning." *ChemBioChem*, 2023.
10. **Özçelik, Rıza**, Alperen Bağ, Berk Atıl, Melih Barsbey, Arzucan Özgür, and Elif Özkırmı. "A Framework for Improving the Generalizability of Drug-Target Affinity Prediction Models." *Journal of Computational Biology*, 2023.
11. Barsbey, Melih, **Rıza Özçelik***, Alperen Bağ, Berk Atıl, Arzucan Özgür, and Elif Özkırmı. "A Computational Software for Training Robust Drug-Target Affinity Prediction Models: pydebiasedtda." *Journal of Computational Biology*, 2023.
12. Budur, Emrah, **Rıza Özçelik**, Dilara Soylu, Omar Khatatab, Tunga Güngör, and Christopher Potts. "Building Efficient and Effective OpenQA Systems for Low-Resource Languages." *Accepted to Knowledge-Based Systems*, 2023.
13. **Özçelik, Rıza***, Hakime Öztürk, Arzucan Özgür, and Elif Ozkirimli. "ChemBoost: A chemical language based approach for the prediction of protein - ligand binding affinity." *Molecular Informatics*, 2021.
14. Budur, Emrah, **Rıza Özçelik**, Tunga Güngör, and Christopher Potts. "Data and Representation for Turkish Language Inference." *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, 2020.
15. Köksal, Abdullatif, Hilal Dönmez, **Rıza Özçelik**, Elif Ozkirimli, and Arzucan Özgür. "Vapur: A Search Engine to Find Related Protein-Compound Pairs in COVID-19 Literature." *Proceedings of the 1st Workshop on NLP for COVID-19 (Part 2) at EMNLP*, 2020.
16. **Özçelik, Rıza**, Gökçe Uludoğan, Selen Parlar, Özge Bakay, Özlem Ergelen and Olcay Taner Yıldız. "User Interface for Turkish Word Network KeNet." *Signal Processing Applications*, 2019.
17. Uludoğan, Gökçe, **Rıza Özçelik**, Selen Parlar, Gökhan Ercan and Olcay Taner Yıldız. "User Interfaces for Turkish Natural Language Processing." *Signal Processing Applications*, 2019.
18. Ercan, Gökhan, Orçun Erkek, Onur Açıkgoz, **Rıza Özçelik**, Selen Parlar and Olcay Taner Yıldız. "Data Set Generation for Analysing of Turkish Semantic and Sentence Similarity." *3rd International Conference on Computer Science and Engineering (UBMK)*, 2018.

Selected Talks & Presentations

- 3 posters at ICML - Machine Learning for Life and Material Science Workshop 2024;
- Selected talk (15min) at Applied Machine Learning Days (2024);
- Invited talk (1h) at M2D2 Talk series (2024);
- Selected talk (15min) at ELLIS ML4Molecules Workshop 2023;
- Selected talk (15min) at World Chemistry Congress (IUPAC-CHAINS) 2023;
- Poster at IEEE Conference on Computational Intelligence in Bioinformatics and Computational Biology 2023;
- Selected talk (5min) at Institute of Complex Molecular Systems Symposium 2023;
- Guest lecturer at TUE Advanced Programming Course 2023;
- Selected talk at RECOMB2023 conference (15min);
- Poster at ICLR - Machine Learning for Drug Discovery Workshop 2022;
- Two selected talks (15min each) at ISMB 2021;
- Two posters at ISMB 2021;
- Selected talk (15min) and poster in HIBIT 2020.

Honors & Awards

- Google EMEA Academic Scholarship;
- Winner at scientific communication contest;
- Three best bachelor thesis awards (as a thesis supervisor);
- Scientific Council of Turkey (TUBITAK) graduate student scholarship;
- Multiple undergraduate scholarships for 5 years.

References

- Assist. Prof. Francesca Grisoni
Dept. of Biomedical Engineering, Eindhoven University of Technology, Eindhoven.
Ph.D. Supervisor. f.grisoni@tue.nl
- Assoc. Prof. Arzucan Özgür
Dept. of Computer Engineering, Boğaziçi University, Istanbul.
BSc. and MSc. Supervisor. arzucan.ozgur@bogazici.edu.tr
- Assoc. Prof. Elif Ozkirimli
Head of Computational Science Products, Roche, Basel, Switzerland.
MSc. Co-supervisor. elif.ozkirimli@roche.com