Rıza Özçelik | Ph.D. candidate

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Education

- 2022–2026: **Ph.D.**, **Biomedical Engineering**, *Eindhoven University of Technology, The Netherlands*.
  Thesis: Reshaping Generative Deep Learning for 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

1. **Özçelik, Rıza**, Francesca Grisoni. "The Jungle of Generative Drug Discovery: Traps, Treasures, and Ways Out." *ArXiv doi: 10.48550/arXiv.2501.05457*, 2025.

2. **Özçelik, Rıza**, Francesca Grisoni. "De Novo Drug Design by Chemical Language Modeling." Book chapter in *An Introduction to Generative Drug Discovery*, 2025.

3. van Weesep, Laura, **Rıza Özçelik***, Marloes Pennings, Luc Brunsveld, Francesca Grisoni. "Exploring 14-3-3 Interactome with Deep Learning." *In preparation*, 2025.

4. **Özçelik, Rıza**, Sarah de Ruiter, Emanuele Crusciolo, and Francesca Grisoni. "Chemical Language Modeling with Structured State Space Sequence Models." *Nature Communications*, 2024.

5. **Özçelik, Rıza**, and Francesca Grisoni. "A Hitchhiker's Guide to Deep Chemical Language Processing for Bioactivity Prediction." *Digital Discovery*, Accepted Manuscript, 2024.

6. **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-v2*, 2024.

7. Birolo, Rebecca, **Rıza Özçelik**, Andrea Aramini, Roberto Gobetto, Michele R. Chierotti, Francesca Grisoni. "Deep Supramolecular Language Processing for Co-crystal Prediction." *ChemRxiv doi: 10.26434/chemrxiv-2024-vgvhk=v3*, 2024.

8. Criscuolo, Emanuele, **Rıza Özçelik**, Derek van Tilborg, Francesca Grisoni. "The surprising ineffectiveness of molecular dynamics coordinates for predicting bioactivity with machine learning" *ChemRxiv doi: 10.26434/chemrxiv-2024-rp81v*, 2024.

9. 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.

10. Multari, Silvia, **Rıza Özçelik**, Angelica Mazzolari, Salvatore Nobile, and Francesca Grisoni. "Predicting Metabolic Reactions with a Molecular Transformer for Drug Design Optimization." *IEEE Conference on Computational Intelligence in Bioinformatics and Computational Biology (CIBCB)*, 2024.

11. 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.

12. **Özçelik, Rıza***, Derek van Tilborg, Jose Jiménez-Luna, and Francesca Grisoni. "Structure-based Drug Discovery with Deep Learning." *ChemBioChem*, 2023.

13. **Özçelik, Rıza**, Alperen Bağ, Berk Atıl, Melih Barsbey, Arzucan Özgür, and Elif Özkırımlı. "A Framework for Improving the Generalizability of Drug-Target Affinity Prediction Models." *Journal of Computational Biology*, 2023.

14. Barsbey, Melih, **Rıza Özçelik***, Alperen Bağ, Berk Atıl, Arzucan Özgür, and Elif Özkırımlı. "A Computational Software for Training Robust Drug-Target Affinity Prediction Models: pydebiaseddta." *Journal of Computational Biology*, 2023.

15. Budur, Emrah, **Rıza Özçelik**, Dilara Soylu, Omar Khattab, Tunga Güngör, and Christopher Potts. "Building Efficient and Effective OpenQA Systems for Low-Resource Languages." *Knowledge-Based Systems*, 2023.

16. **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.

17. 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.

18. 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.

19. **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.

20. Uludoğan, Gökçe, **Rıza Özçelik**, Selen Parlar, Gökhan Ercan and Olcay Taner Yıldız. "User Interfaces for Turkish Natural Language Processing." *Signal Processing Applications*, 2019.

21. Ercan, Gökhan, Orçun Erkek, Onur Açıkgöz, **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

- 1 talk (15min) and 2 posters at ELLIS ML4Molecules Workshop 2024;

- 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

- Best Publication Award of 2024 at the institute (18 contestants);
- Google EMEA Academic Scholarship;
- Winner at scientific communication contest (20 attendees);
- Three best bachelor thesis awards (as a thesis supervisor);
- Scientific Council of Turkey (TUBITAK) graduate student scholarship;
- Multiple undergraduate scholarships for 5 years.

Selected Skills

- Independence
- Deep learning
- Pytorch/Keras/Tensorflow
- Teamwork
- Natural language processing
- Git, Anaconda, Bash
- Verbal/written communication
- Drug discovery
- Matplotlib, seaborn, LaTeX

References

- Assoc. Prof. Francesca Grsioni
  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`