

# Egor Marin

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## WORK EXPERIENCE

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### Machine Learning Scientist

ENPICOM B.V.

May 2024 — Present

*Den Bosch, Netherlands*

- full-cycle ML model development: from literature survey and data collection to reproducible training and deployment
- working with both generative and predictive models for various tasks in the antibody development field

### Open-source software engineer

MDAnalysis via Google Summer of Code

May 2023 — September 2023

*Remote*

- wrote backward-compatible parallelization for molecular dynamics trajectory analysis

### PhD Researcher

University of Groningen

June 2021 — Dec 2023

*Groningen, Netherlands*

- full-cycle membrane protein biochemistry: protein expression, purification, nanodisc reconstitution or crystallization
- processed cryoEM data ( 80 CryoSPARC projects), set up cryoEM data processing & management infrastructure
- supervised a project as a corresponding author: [“Regression-Based Active Learning for Accessible Acceleration of Ultra-Large Library Docking”](#)

### Junior Research Associate

Moscow Institute of Physics and Technology

March 2017 — September 2021

*Moscow, Russia*

- last-mile protein crystallography service: crystal harvesting, data management, synchrotron and XFEL data collection
- refined, analysed and deposited protein structures to PDB (38 structures as of September 2025)
- coordinated data analysis and manuscript preparation

### Scientific Journalist

Moscow Institute of Physics and Technology

Jun 2022 — Aug 2022

*Moscow, Russia*

- wrote press-releases on published papers
- communicated with scientists & media.

## SKILLS

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- **Programming Languages:** Python, bash, Rust, C++, Typescript
- **Python:** uv/ruff/ty🔥, pytest, hypothesis, pydantic, dask
- **Data Science:** polars🐼, huggingface🤗, pandas, numpy, sklearn, skrub
- **Deep Learning:** pytorch, lightning, jax, mlflow
- **ML in biology:** protein language models, diffusion/discrete diffusion/flow matching, AlphaFold/Openfold/Boltz
- **Technologies:** AWS, Docker, SLURM, Modal, Airflow, Github actions
- **Cheminformatics:** RDKit, polaris, molecular docking, structural bioinformatics (MDAnalysis/mdtraj/biotite)

## PUBLICATIONS

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**CryoRhodopsins: a comprehensive characterization of a new clade of microbial rhodopsins from cold environments**, Science Advances

7 July 2025

- Prepared samples for cryoEM (nanodisc reconstitution), processed cryoEM data and organized data collection.

**Regression-Based Active Learning for Accessible Acceleration of Ultra-Large Library Docking**, Journal of Chemical Information and Modeling

29 December 2023

- Proposed the project, supervised the study and wrote manuscript, performed ML benchmarks.

**Custom Design of a Humidifier Chamber for In Meso Crystallization**, Crystal Growth & Design

12 December 2023

- Purified and crystallized protein, performed in meso crystallization, processed data, refined the structure, analyzed cryo-EM data, wrote the manuscript.

**Structural insights into thrombolytic activity of destabilase from medicinal leech**, Scientific Reports

24 April 2023

- Crystallized the protein, collected data, solved the structures, performed molecular dynamics simulations and analyzed the results.

- Structural basis for receptor selectivity and inverse agonism in S1P5 receptors**, Nature Communications 12 August 2022
- Collected data at PAL XFEL, processed SFX data, refined model, performed Alphafold simulations, molecular docking & VLS benchmarks of available S1P models.
- Metabolic fate of human immunoactive sterols in Mycobacterium tuberculosis**, Journal of Molecular Biology 19 February 2021
- Collected crystallography data, supervised model refinement, wrote manuscript
- Structural Aspects of Photopharmacology: Insight into the Binding of Photoswitchable and Photocaged Inhibitors to the Glutamate Transporter Homologue**, Journal of American Chemical Society 15 January 2021
- Did molecular docking of photo-switchable compounds in crystallographic structure and compared docking results with functional data.
- Structure-Based Virtual Screening of Ultra-Large Library Yields Potent Antagonists for a Lipid GPCR**, Biomolecules 3 December 2020
- Prepared small-molecule libraries for docking, did large-scale docking and analyzed the results, wrote manuscript.
- Small-wedge synchrotron and serial XFEL datasets for cysteinyl leukotriene GPCRs**, Scientific Data 12 November 2020
- Organized, annotated and deposited raw data, developed robust re-processing algorithms, wrote manuscript.
- Molecular mechanism of light-driven sodium pumping**, Nature Communications 1 May 2020
- Processed serial synchrotron crystallography data using CrystFEL, deposited raw data.
- Structural basis of ligand selectivity and disease mutations in cysteinyl leukotriene receptors**, Nature Communications 6 December 2019
- Collected small-wedge serial synchrotron crystallography data, processed them, refined, deposited and analyzed structures.
- Structure-based mechanism of cysteinyl leukotriene receptor inhibition by antiasthmatic drugs**, Science Advances 1 October 2019
- Collected synchrotron crystallography data, processed XFEL and synchrotron data, refined, deposited and analyzed structures.
- An outlook on using serial femtosecond crystallography in drug discovery**, Expert Opinion on Drug Discovery 11 June 2019
- Wrote sections about SFX data processing & phasing.
- Structural insights into ion conduction by channelrhodopsin 2**, Science 24 November 2017
- Data collection and processing for both WT and mutant proteins.

## EDUCATION

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- University of Groningen** 2019 — 2023  
*PhD* Groningen, Netherlands
- thesis ‘On the methods of studying protein-ligand interaction dynamics’
  - methods: cryoEM, X-ray crystallography, protein biochemistry, protein biophysics
  - publications in JACS, Crystal Growth & Design, Journal of Cheminformatics & Modelling
- Computer Science Center** 2020 — 2022  
*Full-time extracurricular educational program in computer science* St. Petersburg, Russia
- relevant coursework: Python, C++, Algorithms and data structures, Data science, Intro to Linux systems, Rust
- Moscow Institute of Physics and Technology** 2017 — 2019  
*MSc in applied mathematics and physics* Moscow, Russia
- managed bachelor and master students, created a course on modern protein crystallography
  - publications in Science, Nature Communications, Science Advances, Scientific Data
  - graduated *summa cum laude*
- Moscow Institute of Physics and Technology** 2017 — 2019  
*BSc in applied mathematics and physics* Moscow, Russia
- graduated *magna cum laude*

- related coursework: Calculus I-IV, Linear Algebra I-II, Complex Analysis, Differential Equations I-II, Analytical Mechanics I-II, Thermodynamics.

## EXTRACURRICULAR ACTIVITIES

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### Open-source contributions

Jan 2021 — Present

- [reciprocalspaceship](#): wrote parser for serial crystallography data into binary dataframe-like class
- [ntfy-cryosparc](#): wrote web-server to parse CryoSPARC (tm) notifications and notify appropriate users
- [polars-distance](#): minor contribution to polars plugin for distance calculation

### MDAnalysis Core Developer

February 2025 — Present

- [MDAnalysis Core Developer](#)
  - wrote a [parallel backend](#) for all analysis classes (dask/multiprocessing)
  - added a [DSSP module](#) for native secondary structure assignment
  - currently working on an [MMCIF parser](#) based on [gemmi](#)

### Self-hosting

Jan 2021 — Present

- self-hosting bunch of open-source docker containers under Tailscale VPN

### Data Science Competitions

2018 — Present

- top-10% in Kaggle “Predict Molecular Properties” (public notebooks + gradient boosting on self-written rotationally invariant features)
- top-1 in first round of “Learning How To Smell” at AICrowd
- top-10% in Takeda competition at Signate
- 5th place in Tochka Bank graph ML competition