Egor Marin

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Work Experience

Machine Learning Scientist May 2024 — Present
ENPICOM B.V. *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 May 2023 — September 2023
MDAnalysis via Google Summer of Code *Remote*
- designed and wrote backward-compatible parallelization (dask / multiprocessing) for molecular dynamics trajectory analysis

PhD Researcher June 2021 — Dec 2023
University of Groningen *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 March 2017 — September 2021
Moscow Institute of Physics and Technology *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 Jun 2016 — Aug 2017
Moscow Institute of Physics and Technology *Moscow, Russia*
- wrote press-releases on published papers
- communicated with scientists & media.

Skills

- **Programming Languages**: Python, bash, Rust, C++, Typescript
- **Python**: uv/ruff/ty😈, pytest, hypothesis, pydantic, dask
- **Data Science**: polars🫶, huggingface🤗, pandas, numpy, sklearn, skrub
- **Visualization**: altair, marimo, matplotlib/seaborn/jupyter
- **Deep Learning**: pytorch, lightning, jax, mlflow
- **ML in biology**: protein language models, diffusion/discrete diffusion/flow matching, Alphafold/Openfold/Boltz
- **Structural biology**: cryoEM data processing and structure refinement, X-ray crystallography data collection, processing and refinement
- **Technologies**: AWS, Docker, SLURM, Modal, Airflow, Github actions
- **Cheminformatics**: RDKit, polaris, molecular docking, structural bioinformatics (MDAnalysis/mdtraj/biotite)

Publications

CryoRhodopsins: a comprehensive characterization of a new clade of microbial rhodopsins from cold environments
- *Science Advances*, 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*, 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*, 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*, 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*, 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*, 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*, January 2021
- performed 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*, 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*, November 2020
- organized, annotated and deposited raw data, developed robust re-processing algorithms, wrote manuscript

Molecular mechanism of light-driven sodium pumping,
- *Nature Communications*, 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*, December 2019
- collected small-wedge serial synchrotron crystallography data, refined, deposited, and analyzed structures, wrote the manuscript

Structure-based mechanism of cysteinyl leukotriene receptor inhibition by antiasthmatic drugs,
- *Science Advances*, October 2019
- collected synchrotron crystallography data, processed XFEL and synchrotron data, refined, deposited and analyzed structures, wrote the manuscript

An outlook on using serial femtosecond crystallography in drug discovery,
- *Expert Opinion on Drug Discovery*, June 2019
- wrote sections about SFX data processing and phasing

Structural insights into ion conduction by channelrhodopsin 2,
- *Science*, November 2017
- performed data processing for both WT and mutant proteins

Education

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

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 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