

Education

- 2019–2023 **University of Groningen**, *PhD at the Faculty of Science and Engineering*, Thesis title "On the methods of studying protein-ligand interaction dynamics".
- 2019–2022 **Moscow Institute of Physics and Technology**, *PhD at the Department of General and Applied Physics*, program: Physics and Astronomy, specialization: Biophysics.
- 2020–2021 **Computer Science Center (currently Yandex's Data Analysis School)**.
- 2017–2019 **Moscow Institute of Physics and Technology**, *MSc at the Department of General and Applied Physics*, program: Molecular Biology and Biophysics, *GPA – 8.7/10*, diploma "Structural studies of lipid G-protein coupled receptors".
- 2013–2017 **Moscow Institute of Physics and Technology**, *BSc at the Department of General and Applied Physics*, program: biophysics, diploma "Serial synchrotron crystallography of membrane proteins" (BSc with excellence), *GPA – 8.5/10*.

Work & research experience

- May 2024 – ongoing **Machine Learning Scientist**, *ENPICOM B.V.*, Den Bosch, Netherlands.
Design machine learning algorithms for antibody property prediction and optimization, supervise interns, curate internal datasets for antibody structure-property relationship
- May 2023 – Sep 2023 **Software engineer**, *Google Summer of Code, MDAnalysis*, Supervisors: Oliver Beckstein, Richard Gowers, Rocco Meli, Yuxuan Zhuang, Ian Kenney, Remote.
Implemented parallel backend for the MDAnalysis open-source library
- 2021–2023 **PhD student**, *Faculty of Science and Engineering*, Supervisor: Albert Guskov, Groningen.
Membrane protein expression and purification in *E. Coli*, crystal harvesting, data collection at synchrotrons in serial and single-crystal regime. Sample preparation for cryoEM and subsequent data processing. Setup of the cryoEM data processing server (cryoSPARC/RELION).
- 2017–2022 **Researcher**, *Laboratory for advanced studies of membrane proteins*, Supervisor: Valentin Borshchevskiy, Moscow.
Serial and single-crystal synchrotron protein data collection and processing (over 40 shifts at ID23-1, ID29-1, ID30a3, ID30b and BM30 MX beamlines at ESRF, Grenoble, P13, P14 at Petra3, Hamburg, PXI-II at SLS and Proxima-2a at SOLEIL), structure solution and refinement, crystal harvesting and protein crystallization for membrane proteins with LCP, and for soluble proteins. Participated in SFX experiments at PAL XFEL and European XFEL, processed data from LCLS, PAL XFEL and EuXFEL
- Sep-Oct 2019 **Visiting research assistant**, *Groningen University, Guskov lab*, Supervisor: Dr. Albert Guskov, Groningen.
Jan-Feb 2020 Did membrane protein purification & set up LCP crystallization screening
- June-Sep 2018 **Visiting research assistant**, *USC, Katrich lab*, Supervisor: Dr. Vsevolod Katrich, Los Angeles.
Structural bioinformatics & VLS campaigns for G-protein coupled receptors
- Sep 2017 **Trainee**, *CFEL*, Supervisor: Dr. Thomas A. White, Hamburg.
SFX data processing; developing of CrystFEL-based tools (with Python & bash) for SFX data processing and analysis
- 2016 summer **Trainee**, *DESY Summerstudent Program*, Supervisor: Dmitriy Novikov, Hamburg.
Python scripting for X-ray standing wave fluorescence data analysis for bilayer lipid membranes

Skills

Lab structural biology	Membrane protein expression and purification, nanodisc reconstitution, crystallization of soluble proteins (including seeding), crystallization of membrane proteins in LCP, harvesting and synchrotron data collection for all above mentioned
Serial femtosecond crystallography	Processing of native and anomalous data using CrystFEL (from LCLS, PAL XFEL and European XFEL), 7 datasets total (see 6RZ5 structure)
Macromolecular crystallography	Single-crystal and serial synchrotron crystallography data collection (ca. 400 hours of synchrotron beamtime), processing using XDS and XSCALE with particular focus on serial (10's of crystals) approach for challenging targets (see 6EID, 6EIG structures). For 100's of crystals see 6RZ6, also 6RZ7, 6RZ8 and 6RZ9)
cryo-EM	Data processing using CryoSPARC/RELION, model building and refinement using ccpem and Coot
Protein structure solution and refinement	Use of Phenix, CCP4, autoBUSTER and Coot for protein structure solution and refinement)
Structural bioinformatics & docking	Used ICM Molsoft software package for structure analysis, docking and VLS campaign applied to G-protein coupled receptors, protein-protein docking using ZDOCK & its custom analysis
Python	Bag of words: numpy/pytorch/jax, lightning/flax, sklearn/skrubs, polars/patito, huggingface, uv/ruff/ty, pytest
Deep learning	Bag of words: BERT, RoBERTa, DPLM, D3PM, MDLM, UDM, diffusion, discrete diffusion, FUDGE, AlphaFold/Boltz/SAFE
Linux & HPC	git/github, Ubuntu, ubuntu & centos (setup and manage \approx 10 workstations and 3 clusters for high-CPU/high-GPU tasks), self-hosting (docker/podman/ansible/just/task)
2015–2016	Scientific journalist , <i>MIPT PR-team</i> , Moscow. News monitoring & writing explainers on MIPT-affiliated papers, preparing interviews and features

Conferences & Schools

1-3 Sep 2025	Computational Structural Immunology Symposium , <i>Nijmegen, Netherlands</i> , Participant. Symposium on computational immunology
2-9 Sep 2022	ASPP School , <i>Bilbao, Spain</i> , Participant. Scientific programming school
23-25 Jan 2019	European XFEL User Meeting , <i>Hamburg, Germany</i> , Participant. Fruitful discussions regarding our preceeding experiment at European XFEL
30 Nov - 1 Dec 2017	EUCALL Workshop: Biology at Advanced Laser Light Sources , <i>Hamburg, Germany</i> , Participant. Poster on "Improvements in Serial Femtosecond Crystallography via Multiple Hits Indexing and Peak Search Adjustment"
3-11 Nov. 2017	The 5th Annual iHuman Forum , <i>Shanghai, China</i> , Participant. Poster on "Improvements in Serial Femtosecond Crystallography via Multiple Hits Indexing and Peak Search Adjustment"
2-11 Jun. 2017	International School of Crystallography: Integrative Structural Biology , <i>Et-tore Majorana Foundation and Centre for Scientific Culture</i> , Participant. Poster "Serial Synchrotron Crystallography of G-protein Coupled Receptors"
9-11 Jan. 2017	CCP4 Study Weekend , <i>Science and Technology Facilities Council</i> , Participant. Focus on extitde novo phasing methods; extensive "Validation" section

Scholarships & Awards

Successful Grants & Proposals

- 2019 **GCP research grant for academics (\$5000, proposal author)**, *Grant for support of XFEL-SFX and SSX data processign using Google Cloud computing architecture*, Proposal author.

Publications

- Science Advances **CryoRhodopsins: a comprehensive characterization of a new clade of microbial rhodopsins from cold environments**, Gerrit HU Lamm, **E. Marin**, ... A. Guskov, K. Kovalev, 7 July 2025.
Prepared samples for cryoEM (nanodisc reconstitution), processed cryoEM data and organized data collection.
- bioRxiv **Structural basis for no retinal binding in flotillin-associated rhodopsins**, K. Kovalev, A. Stetsenko, F. Trunk, **E. Marin**, ... A. Guskov, K. Kovalev, 29 April 2025.
Prepared samples for cryoEM (nanodisc reconstitution), processed cryoEM data and organized data collection.
- Nature Communications **A subgroup of light-driven sodium pumps with an additional Schiff base counterion**, E. Podoliak, GHU. Lamm, **E. Marin**, ... K. Kovalev, 4 October 2024.
Reconstituted protein into nanodiscs and processed cryo-EM data.
- Journal of Chemical Information and Modeling **Regression-Based Active Learning for Accessible Acceleration of Ultra-Large Library Docking**, **E. Marin**, M. Kovaleva, ... A. Guskov, V. Borshchevskiy, 29 December 2023.
Proposed the project, supervised the study and wrote manuscript, performed ML benchmarks.
- Crystal Growth & Design **Custom Design of a Humidifier Chamber for *In Meso* Crystallization**, **E. Marin**, K. Kovalev, ... V. Borshchevskiy, A. Guskov, 12 December 2023.
Purified and crystallized protein, performed *in meso* crystallization, processed data, refined the structure, analyzed cryo-EM data, wrote the manuscript.
- Nature Comm. Chemistry **Mirror proteorhodopsins**, N. Malyar, K. Kovalev, ... E. Bamberg, V. Gordeliy, 2 May 2023.
Collected crystallographic data and solved the structure.
- Scientific Reports **Structural insights into thrombolytic activity of destabilase from medicinal leech**, **E. Marin**, D. A. Kornilov, ... V. Borshchevskiy, 24 April 2023.
Crystallized the protein, collected data, solved the structures, performed molecular dynamics simulations and analyzed the results.
- Acta Crystallographica Section D **Structural insights into the effects of glycerol on ligand binding to cytochrome P450**, S. Bukhdruker, ... V. Borshchevskiy, 12 August 2022.
Collected data at PAL XFEL, processed SFX data, refined model, performed AlphaFold simulations, molecular docking & VLS benchmarks of available S1P models
- Nature Communications **Structural basis for receptor selectivity and inverse agonism in S1P5 receptors**, E. Lyapina, A. Gusach, **E. Marin**, ... V. Cherezov, 12 August 2022.
Collected data at PAL XFEL, processed SFX data, refined model, performed AlphaFold simulations, molecular docking & VLS benchmarks of available S1P models
- Bioorganic Chemistry **A new twist of rubredoxin function in M. tuberculosis**, T. Sushko, ... A. Gilep, N. Strushkevich, 1 April 2021.
Collected crystallography data, supervised model refinement, discussed draft
- Journal of Molecular Biology **Metabolic fate of human immunoactive sterols in Mycobacterium tuberculosis**, T. Varaksa, ... V. Borshchevskiy, N. Strushkevich, 19 February 2021.
Collected crystallography data, supervised model refinement, discussed draft

Journal of American Chemical Society	<p>Structural Aspects of Photopharmacology: Insight into the Binding of Photoswitchable and Photocaged Inhibitors to the Glutamate Transporter Homologue, V. Arkhipova, ..., W. Szymanski, D. J. Slotboom, A. Guskov, 15 January 2021.</p> <p>Did molecular docking of photo-switchable compounds in crystallographic structure and compared docking results with functional data</p>
Biomolecules	<p>Structure-Based Virtual Screening of Ultra-Large Library Yields Potent Antagonists for a Lipid GPCR, A. Sadybekov, R. Brouillette, E. Marin, ..., P. Sarret, V. Katritch, 3 December 2020.</p> <p>Prepared small-molecule libraries for docking, did large-scale docking and analyzed the results, wrote manuscript</p>
International Journal of Molecular Sciences	<p>Hydroxylation of antitubercular drug candidate, SQ109, by mycobacterial cytochrome P450, S. Bukhdruker, ..., V. Borshchevskiy, N. Strushkevich, 16 October 2020.</p> <p>Collected crystallography data, supervised model refinement, discussed draft</p>
Scientific Data	<p>Small-wedge synchrotron and serial XFEL datasets for cysteinyl leukotriene GPCRs, E. Marin, ..., V. Cherezov, V. Borshchevskiy, 12 November 2020.</p> <p>Organized, annotated and deposited raw data, developed robust re-processing algorithms, wrote manuscript</p>
Nature Communications	<p>Molecular mechanism of light-driven sodium pumping, K. Kovalev, ..., E. Bamberg, V. Gordeliy, Published 1 May 2020, 10.1038/s41467-020-16032-y.</p> <p>Processed serial synchrotron crystallography data using CrystFEL, deposited raw data</p>
Nature Communications	<p>Structural basis of ligand selectivity and disease mutations in cysteinyl leukotriene receptors, A. Gusach, A. Luginina, E. Marin, ..., V. Katritch, ..., V. Cherezov, Published 6 December 2019, doi:10.1038/s41467-019-13348-2.</p> <p>Collected small-wedge serial synchrotron crystallography data, processed them, refined, deposited and analyzed structures</p>
Science Advances	<p>Structure-based mechanism of cysteinyl leukotriene receptor inhibition by antiasthmatic drugs, A. Luginina, A. Gusach, E. Marin, ..., V. Katritch, V. Borshchevskiy, V. Cherezov, Published 1 October 2019, doi:10.1126/sciadv.aax2518.</p> <p>Collected synchrotron crystallography data, processed XFEL and synchrotron data, refined, deposited and analyzed structures</p>
Expert Opinion on Drug Discovery	<p>An outlook on using serial femtosecond crystallography in drug discovery, A. Mishin, ..., V. Cherezov, Published 11 June 2019, doi:10.1080/17460441.2019.1626822.</p> <p>Wrote sections about SFX data processing & phasing</p>
Science	<p>Structural insights into ion conduction by channelrhodopsin 2, O. Volkov, K. Kovalev, V. Polovinkin, V. Borshchevskiy, ..., E. Bamberg, V. Gordeliy, Published 24 November 2017, doi:10.1126/science.aan8862.</p> <p>Data collection and processing for both WT and mutant proteins</p>
Journal of Physics D: Applied Physics	<p>Element-specific density profiles in interacting biomembrane models, E. Schneck, ..., G. Gochev, Published 9 February 2017, doi:10.1088/1361-6463/aa59d3.</p>