Dr. Aleksandra Ivanova (formerly Nikonenko)

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Profile

Computational chemist with strong experience in **computer-aided drug design**, **molecular modeling**, **cheminformatics**, and **scientific software development**. My work combines molecular docking, molecular dynamics simulations, binding free-energy analysis, QSAR, *de novo* molecular design, Python-based workflow automation, and HPC execution for small-molecule drug discovery. **Lead developer** of StreaMD (★ 100+ 20+), an open-source toolkit for automated setup, execution, and analysis of molecular dynamics simulations at scale.

Skills

Programming	`Python`, `Bash`, `R`, `Cython`, `SQL`, LaTeX
Drug discovery/CADD	Molecular docking, molecular dynamics simulations, binding free-energy calculations (GBSA/PBSA/FEP/ABFE), QSAR *de novo* design, protein–ligand interaction analysis, automated preprocessing and quality control of chemical datasets
Cheminformatics	`RDKit`, `MDAnalysis`, `ProLIF`, `CReM`, `GROMACS`, `OpenMM`, `Amber`, `AutoDock Vina`, `Gnina`, `Glide`, `Maestro`, `gmx_MMPBSA`, `A3FE`, `ChemFP`, `Gaussian`, `MCPB.py`, `PyMOL`, `Chimera`
Python ecosystem	`scikit-learn`, `pandas`, `NumPy`, `Matplotlib`, `Plotly`, `Streamlit`
High-performance computing	`Dask`, `PBS`, `SLURM`, `multiprocessing`, `parallel`, code performance profiling
Software development	Git/GitHub, package distribution (`PyPI`, `conda-forge`), environment management (`conda`, `venv`), containerization (`Docker`, `Apptainer`), REST API design, construction of reproducible workflows, unit testing, integration testing
LLMs/AI agents	Development of agent-driven scientific workflows; hands-on experience with hosted and local/open-source LLMs, prompt design, tool integration, and structured agent–tool communication

Experience

2026–present — **Researcher** Institute of Molecular and Translational Medicine, Palacký University, Czech Republic
Conduct computational drug discovery research involving molecular dynamics simulations, molecular docking, binding free-energy analysis, QSAR modeling, and *de novo* molecular design. Develop Python-based workflows and open-source tools for reproducible molecular modeling, including `StreaMD` and `CReM-opt`.

Jun–Dec 2022 — **Computer Scientist (part-time)** AI|ffinity s.r.o, Czech Republic
Curated and validated protein structure (PDB) datasets for MD and ML pipelines; performed molecular docking using Glide.

2017–2019 — **Laboratory Assistant** Laboratory of Chemistry and Biochemistry, Volgograd State University, Russia
Provided laboratory assistance in chemistry and biochemistry, including sample preparation, handling laboratory equipment, maintaining laboratory materials, and supporting routine experimental procedures.

Education

2019–2026 — **Ph.D., Molecular and Translational Medicine — Computational Chemistry** Palacký University, Czech Republic
Thesis: *From molecular conformation to biological activity: computational methods for the design of small molecules*. Supervisor: Dr. Pavel Polishchuk

2014–2019 — **Specialist (Honours), Bioengineering & Bioinformatics** Volgograd State University, Russia

Projects

Lead Developer

CReM-agent
Developed an autonomous, agent-driven molecular optimization framework powered by CReM and molecular docking. *Manuscript in preparation*.

StreaMD ★ 100+ ⑂ 20+ GitHub
Developed an open-source toolkit for automated setup, execution, and analysis of high-throughput molecular dynamics simulations. Published in *J. Cheminformatics* (2024). *First-author publication*.

CReM-opt GitHub
Developed a docking-guided molecular optimization framework combining CReM fragment replacement, genetic algorithm, an AI agent, and atom-wise docking score attribution. Presented at *RDKit UGM 2025*. Poster Award at *12th ICCS 2022, Netherlands*. *Manuscript in preparation*.

MIL-based QSAR Modeling
Developed a conformer-based multi-instance learning approach for molecular activity prediction. Automated the collection of activity-cliff datasets (stereoisomers with differential biological activity). *First-author publication*. Contributed to a related study through dataset curation and molecular docking.

ChEMBL Datasets Collection GitHub
Developed an automated pipeline for retrieving and preprocessing bioactivity datasets from ChEMBL, tailored to specific activity types (e.g., agonists, antagonists, inverse agonists).

HPC Stats Scripts GitHub
Developed utilities for monitoring `SLURM`/`PBS` job efficiency and CPU/GPU/memory usage in HPC environments.

Selected Research Contributions

CACHE Challenge #1 — 3rd Place Team WDR Domain of LRRK2
Developed and applied a docking-guided *de novo* molecule generation workflow using `CReM-opt` and performed MD-based evaluation of identified hits.

Tubulin Inhibitor SAR Studies co-author of 4 publications
Performed molecular docking, molecular dynamics simulations, free energy calculations, `ProLIF`-based protein–ligand interaction analysis, parameterization of boron-containing molecules using `Gaussian`.

EasyDock GitHub
Implemented a Python-based `AutoDock Vina` workflow as part of a scalable molecular docking tool.

Selected Publications

9 total — full list on ORCiD

- A. **Ivanova**, O. Mokshyna, and P. Polishchuk. “StreaMD: the toolkit for high-throughput molecular dynamics simulations”. In: *Journal of Cheminformatics* (2024). DOI: 10.1186/s13321-024-00918-w
- A. **Nikonenko** et al. “Multiple Conformer Descriptors for QSAR Modeling”. In: *Molecular Informatics* (2021). DOI: 10.1002/minf.202060030
- F. Li et al. (incl. **Ivanova** A.). “CACHE Challenge #1: Targeting the WDR Domain of LRRK2, A Parkinson’s Disease Associated Protein”. In: *Journal of Chemical Information and Modeling* (2024). DOI: 10.1021/acs.jcim.4c01267

Honors & Awards

2026 — **3rd Place (individual on-site entry)** *in silico* Drug Design Challenge, Olomouc, Czech Republic
Workshop "Advanced *in silico* Drug Design"

2022/2025 — **Dean’s Award** Palacký University
Significant publication activity 2021/2024 — "Multiple Conformer descriptors for QSAR modeling", "StreaMD: the toolkit for high-throughput molecular dynamics simulations"

2023 — **3rd Place Team** CACHE Challenge #1
Prediction and experimental validation of hits for WDR domain of LRRK2

2022 — **Poster Award** 12th ICCS, Netherlands
GenCReM: *de novo* molecular generation

Lectures & Workshops

2023–2026 — **Lecturer, annual workshop "Advanced *in silico* Drug Design"**
Palacký University, Olomouc, Czech Republic
Molecular Dynamics Workshop

2025 — **Talk, RDKit UGM 2025** Prague, Czech Republic
CReM-opt: *de novo* design guided by explainable docking