Pavlo Polishchuk, PhD, Dr. habil.

Associate Professor | Head, Chemoinformatics and Drug Design Group

Institute of Molecular and Translational Medicine, Faculty of Medicine and Dentistry, Palacký University Olomouc
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Group: imtm.cz/laboratories/chemoinformatics-and-drug-design | **Group GitHub:** github.com/ci-lab-cz
Scopus: scopus.com/authid/detail.uri?authorId=6507794566 | **Personal website:** qsar4u.com

Professional Profile

Computational chemist and research-group leader specializing in cheminformatics, computer-aided drug design, de novo molecular generation, molecular docking, pharmacophore modeling, explainable machine learning, and automated molecular simulations. Developer of the CReM ecosystem, EasyDock, pmapper, SPCI, SiRMS, and StreaMD. Principal investigator of international research projects with a combined budget of EUR 770,000 and author of 85 peer-reviewed journal articles. Research integrates methodological development, open-source software, high-performance computing, and prospective molecular discovery.

Core expertise: de novo design • molecular docking • molecular dynamics and binding free energy • QSAR/QSPR • pharmacophore modeling • machine learning and multi-instance learning • cheminformatics software development

85 peer-reviewed journal articles	**5** book chapters	**2400+** citations
EUR 770k competitive funding as PI	**10+** open-source software packages	**61,744** PyPI downloads excluding mirrors 22 Jan–21 Jul 2026

Current Appointments

2022–present — **Head, Chemoinformatics and Drug Design Group**
Institute of Molecular and Translational Medicine, Palacký University Olomouc, Czech Republic

2015–present — **Senior Researcher**
Institute of Molecular and Translational Medicine, Palacký University Olomouc, Czech Republic

Education and Academic Qualifications

2026 — **Associate Professor title**
Palacký University Olomouc, Czech Republic

2024 — **Dr. habil.**
University of Strasbourg, France. Habilitation thesis: “New methodologies of machine learning modeling of complex chemical systems: mixtures, reactions and ligand–protein complexes.”

2009 — **PhD in Bioorganic Chemistry**
A. V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine, Odesa. Thesis: “Affinity of 5-HT1A receptors to their ligands: QSAR analysis toward a hierarchical system of models based on simplex molecular representation.” Supervisor: Prof. V. E. Kuz’min.

1996–2001 — **Master’s degree in Chemistry**
Odesa National University, Ukraine

Research Leadership and Competitive Funding

2023–2026 — **LUAUS23262 — De Novo Design of Synthetically Feasible Compounds Guided by Artificial Intelligence**
INTER-EXCELLENCE II / INTER-ACTION, Ministry of Education, Youth and Sports, Czech Republic. Role: Principal Investigator. Total funding: EUR 470,000.

2018–2020 — **LTARF18013 — Improving the Output of Primary Screening of Biologically Active Compounds Using Computational Models**
INTER-EXCELLENCE / INTER-ACTION, Ministry of Education, Youth and Sports, Czech Republic. Role: Principal Investigator. Total funding: EUR 300,000.

Selected Scientific Contributions

- **Fragment-based de novo molecular design.** Developed CReM, a framework for structure generation through chemically reasonable fragment transformations. The approach provides indirect control over synthetic accessibility and supports hit discovery, lead optimization, scaffold hopping, fragment expansion, and scaffold decoration. It has been extended into docking-, pharmacophore-, and machine-learning-guided workflows, including CReM-dock, CReM-pharm, CReM-opt, and CReM-ML.
- **Open-source automated drug-discovery workflows.** Led the development of EasyDock for automated and distributed high-throughput molecular docking and StreaMD for automated molecular dynamics and binding free-energy calculations. These tools provide modular, reproducible workflows suitable for high-performance computing and integration into larger design pipelines.

- **Three-dimensional pharmacophore modeling and multi-instance learning.** Developed stereosensitive pharmacophore representations and conformer-ensemble modeling approaches that treat molecules as sets of interconvertible structures rather than single conformations. These methods support molecular similarity, pharmacophore search, QSAR modeling, and identification of biologically relevant conformers.
- **Explainable QSAR and knowledge extraction.** Developed SPCI, a model-independent framework for deriving atom- and fragment-level contributions from QSAR/QSPR models. The method converts statistical models into interpretable structure–property relationships that can guide molecular optimization and structural-alert analysis.
- **Representation of complex chemical systems.** Developed descriptor-based approaches for modeling mixtures of arbitrary composition and chemical reactions, together with methods for interpreting nonlinear Random Forest QSAR models.

Open-Source Software and Research Infrastructure

Platform	Scope
CReM	Fragment-based structure generation through chemically reasonable mutations; de novo design, optimization, scaffold hopping and decoration.
CReM-dock	Docking-guided de novo design and fragment expansion with control of synthetic accessibility and protein-ligand interactions.
CReM-pharm	Pharmacophore-guided de novo design with synthetic-accessibility awareness.
EasyDock	Automated, customizable and distributed high-throughput molecular docking.
StreaMD	Automated molecular dynamics and binding free-energy workflows.
pmapper	Perception, encoding, manipulation and comparison of 3D pharmacophores.
SPCI	Model-independent structural and physicochemical interpretation of QSAR/QSPR models.
SiRMS	Fast calculation of simplex descriptors for compounds, mixtures, quasi-mixtures and reactions.

Additional software: psearch, pharmd, 3D-MIL-QSAR, i-benchmarks, and CF. The PyPI packages listed in this CV received 61,744 downloads excluding mirrors during 22 January–21 July 2026.

Selected Publications

1. Minibaeva, G.; Du, H.; Clark, F.; Michel, J.; **Polishchuk, P.** CReM-dock: de novo design of synthetically feasible structures guided by molecular docking. *Digital Discovery* 2026, 5, 2271–2291. DOI: 10.1039/D6DD00131A

2. Denzler, A.; Sriramulu, D. K.; Pecha, J.; **Polishchuk, P.** CReM-pharm: de novo 3D pharmacophore-based design with synthetic accessibility awareness. *Journal of Cheminformatics* 2026, 18, 70. DOI: 10.1186/s13321-026-01195-5

3. Zankov, D.; Madzhidov, T.; Varnek, A.; **Polishchuk, P.** Chemical complexity challenge: Is multi-instance machine learning a solution? *WIREs Computational Molecular Science* 2024, 14 (1), e1698. DOI: 10.1002/wcms.1698

4. Minibaeva, G.; Ivanova (Nikonenko), A.; **Polishchuk, P.** EasyDock: customizable and scalable docking tool. *Journal of Cheminformatics* 2023, 15, 102. DOI: 10.1186/s13321-023-00772-2

5. Zankov, D. V.; Matveieva, M.; Nikonenko, A. V.; Nugmanov, R. I.; Baskin, I. I.; Varnek, A.; **Polishchuk, P.**; Madzhidov, T. I. QSAR modeling based on conformation ensembles using a multi-instance learning approach. *Journal of Chemical Information and Modeling* 2021, 61, 4913–4923. DOI: 10.1021/acs.jcim.1c00692

6. Polishchuk, P. CReM: chemically reasonable mutations framework for structure generation. *Journal of Cheminformatics* 2020, 12, 28. DOI: 10.1186/s13321-020-00431-w

7. Polishchuk, P. Interpretation of Quantitative Structure–Activity Relationship Models: Past, Present, and Future. *Journal of Chemical Information and Modeling* 2017, 57 (11), 2618-2639. DOI: 10.1021/acs.jcim.7b00274

Publication record: 85 peer-reviewed journal articles, 5 book chapters and more than 100 conference contributions. Complete records are available through ORCID and Scopus.

Doctoral Supervision

2021–present — **Guzel Minibaeva**
"De novo design of synthetically feasible compounds."

2019–2026 — **Aleksandra Nikonenko**
"From molecular conformation to biological activity: computational methods for the design of small molecules."

2019–2025 — **Alina Kutlushina**
"Development of 3D pharmacophore signatures and their application in drug design." Studies discontinued in 2025.

2016–2022 — **Mariia Matveieva**
"Automatic mining of structure–activity relationships from chemical datasets."

Other Research Supervision and Mentoring

- **Master's and bachelor's students.** Dávid Švec (2016–2019), data-driven optimization of compound properties and chemical-space exploration; Andrea Dobešová (2026–present), analysis of chemically induced cellular morphology.

- **Erasmus+ students.** Tereza Kubatová, University of Vienna (2024), multi-instance models for biologically relevant conformers; Marta Pitarch Savall, University of Lleida (2025), Cell Painting analysis of bioactive alkaloids; Stanislav Tricolici, IMC Krems (2025–2026), machine-learning prioritization of fragments for de novo design.
- **Research interns and trainees.** Michal Sobieraj (2025), consensus QSPR and key-conformer identification; Anna Siskova (2025–present), morphological profiling of chemical compounds; Elena Mokshina, Tetiana Khristova, Oleg Tin'kov, and Maxim Kulinskiy (2010–2014), QSAR/QSPR and computational drug-design projects.

Teaching and Workshop Organization

2017–2026 **Co-organizer and Lecturer, Advanced In Silico Drug Design Workshop**
Annual international workshop at Palacký University Olomouc; eight editions covering cheminformatics, molecular docking, machine learning, molecular dynamics and free-energy calculations.

2024 **Invited Professor, University of Strasbourg**
Teaching visit, 21 October–2 November 2024.

2016–present **Rational Drug Design course**
Lectures at Palacký University Olomouc.

2014 **Introduction to R and Modeling with R**
Lectures and tutorials, A. V. Bogatsky Physico-Chemical Institute, Odesa.

2013 **Computer-Aided Drug Development**
Lectures on structure- and ligand-based approaches, University of Silesia, Katowice.

2010 **Computer-Aided Drug Design**
Lectures, Odesa National University.

Teaching resources: Advanced In Silico Drug Design | QSAR4U tutorials

Selected Keynote, Plenary and Invited Lectures

2025 **Invited Lecturer, Erasmus Mundus Summer School on Chemoinformatics, Ljubljana**
"Multi-instance learning as a response to the complexity of molecular entities."

2024 **Keynote Speaker, 8th IT4Innovations Users' Conference, Ostrava**
"StreaMD: high-throughput automated molecular dynamics simulations tool."

2024 **Invited Speaker, In Silico Design Forum, Johnson & Johnson**
"De novo design and optimization."

2024 **Plenary Speaker, 9th Strasbourg Summer School on Chemoinformatics**
"Multi-instance learning as a response to the complexity of molecular entities."

2024 **Invited Speaker, CACHE Symposium, Toronto**

2024 **Invited Lecturer, University of Strasbourg**
"Multi-instance learning as a response to complexity of chemical systems."

2023 **Keynote Speaker, 7th IT4Innovations Users' Conference, Ostrava**
"The first CACHE challenge: searching for hit molecules in ultra-large chemical databases."

2023 **Invited Lecturer, University of Vienna**
"The first CACHE challenge: searching for hit molecules in ultra-large chemical databases."

2022 **Plenary Speaker, Strasbourg Summer School on Chemoinformatics**
"Explainable artificial intelligence: evolution, achievements and perspectives."

2019 **Invited Speaker, Mendeleev Congress, St Petersburg**
"Chemical library design: revisiting the Lipinski rule."

Previous Employment and Professional Experience

2022–2025 **Scientific Advisor and Mentor**
AI|ffinity, Brno, Czech Republic

2014–2015 **Senior Researcher**
A. V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine, Odesa.

2010–2014 **Research Scientist**
A. V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine, Odesa.

2011–2012 **Invited Researcher**
Laboratory of Chemoinformatics, University of Strasbourg, France.

2009–2015 **Member and Consultant, First-Level Quality-Control Team**
Reaxys Database, Elsevier.

2004–2010 **Junior Researcher**
A. V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine, Odesa.

2002–2009 **Patent Data Extraction and Curation**
Reaxys Database, MDL/Elsevier.

2000–2001 **Engineer**
A. V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine, Odesa.

Editorial and Professional Service

- Editorial Board Member, *Molecular Informatics* (from 2026).
- Guest Editor, *Pharmaceuticals*, Special Issue "Pharmacophore Modeling and Applications in Drug Discovery: Challenges and Recent Advances."
- **Peer reviewer for more than 20 international journals, including** *Nature Machine Intelligence*, *Angewandte Chemie International Edition*, *ACS Central Science*, *Journal of Medicinal Chemistry*, *Journal of Chemical Information and Modeling*, *Journal of Cheminformatics*.
- **Member of PhD defence committees:** Martin Šícho, University of Chemistry and Technology Prague (2021); Wim Dehaen, University of Chemistry and Technology Prague (2024).

Honours and Awards

2021, 2024, 2025	**Dean's Awards for Significant Publication Activity** Faculty of Medicine and Dentistry, Palacký University Olomouc; awarded for publication activity in 2020, 2023 and 2024.
2013	**Winner, Innovative Projects Competition** Odesa Innovative Information Centre INVAC; project on the development of platelet-aggregation inhibitors as prospective cardiovascular drugs.
2012	**Short-Term Scholarship** French Embassy in Ukraine, programme for young scientists.
2009–2011	**Scholarship for Young Scientists** National Academy of Sciences of Ukraine.

Languages

Russian, **Ukrainian, English** — fluent | **Czech** — intermediate